Optimization of salt dependent RNA nearest-neighbor enthalpy and entropy parameters

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Supplementary Tabs. S1–S5 show the sequences and their measured temperatures at different species concentrations used to calculate the optimized parameters. The validation sequences are shown in Tab. S6. Regression coefficients for the quadratic interpolations are given in supplementary Tabs. S7 and S8. Supplementary Figs. S1–S4 show the scatter plots of the predicted and experimental melting temperatures.

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Table S1: Sequences for data set `D-RW-71`, shown are the experimental temperatures T_{exp} and corresponding predictions.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
CUGCAG/GACGUC	8.18	29.09	27.6276	27.5804
(repeated)	15.8	31.13	29.8168	29.7623
(repeated)	26.6	32.66	31.5718	31.5113
(repeated)	46	34.54	33.4392	33.3723
(repeated)	78.2	36.23	35.2703	35.197
(repeated)	126	37.81	36.9351	36.856
(repeated)	214	38.7	38.805	38.7193
(repeated)	386	41.93	40.9139	40.8208
(repeated)	651	44	42.8067	42.7066
GCGCGC/CGCGCG	9.02	46.78	47.3487	47.2289
(repeated)	10.5	47.17	47.8545	47.7416
(repeated)	12.4	46.76	48.4102	48.3046
(repeated)	15.7	47.82	49.2018	49.1069
(repeated)	19.5	49.24	49.9324	49.8474
(repeated)	20.9	50.16	50.1668	50.0849
(repeated)	25.1	50.04	50.7875	50.7141
(repeated)	27.5	50.46	51.098	51.0287
(repeated)	48.1	52.88	53.0116	52.9687
(repeated)	80.1	54.75	54.7771	54.7586
(repeated)	104	55.56	55.6884	55.6826
(repeated)	126	56	56.3613	56.3651
(repeated)	204	57.81	58.0633	58.0911
(repeated)	371	60.25	60.2005	60.2589
(repeated)	626	61.8	62.0926	62.1785
CAGCUG/GUCGAC	6.96	26.13	27.0953	27.0498
(repeated)	12	27.67	28.8981	28.8466
(repeated)	22.1	29.96	30.945	30.8867
(repeated)	70.4	34.29	34.9059	34.834
(repeated)	126	36.49	36.9351	36.856
(repeated)	178	37.28	38.1522	38.0689
(repeated)	322	38.99	40.2627	40.1719
(repeated)	674	42.21	42.9332	42.8327
CGGCCG/GCCGGC	8.16	45.45	46.4631	46.31
(repeated)	8.73	46.25	46.6962	46.547
(repeated)	16.6	48.62	48.932	48.8197
(repeated)	22.6	49.64	50.0166	49.9225
(repeated)	31.2	50.75	51.158	51.0831
(repeated)	86.6	54.8	54.8252	54.813
(repeated)	91.5	55.31	55.0252	55.0165
(repeated)	106	54.97	55.5612	55.5617
(repeated)	168	57.31	57.2503	57.2804
(repeated)	307	59.69	59.488	59.5576
(repeated)	526	61.52	61.5124	61.6182
GCAUGC/CGUACG	8.75	29.41	29.2242	29.2667
(repeated)	15.3	31.39	31.0446	31.0915
(repeated)	26.9	33.43	32.9053	32.9567
(repeated)	49.1	35.17	34.9147	34.9711

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Table S1: (continued) Sequences for data set `D-RW-71`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	83.7	37.01	36.718	36.779
(repeated)	141	39.28	38.5018	38.5673
(repeated)	229	40.55	40.1791	40.2488
(repeated)	408	42.58	42.2003	42.2752
(repeated)	737	45.12	44.2969	44.3773
CGCGCG/GCGCGC	9.11	42.46	42.3329	42.3166
(repeated)	10.8	43.26	42.9205	42.9081
(repeated)	12.2	43.58	43.3426	43.3331
(repeated)	16.7	44.88	44.4353	44.4333
(repeated)	20.5	45.51	45.1528	45.1559
(repeated)	25	45.73	45.8505	45.8584
(repeated)	27.8	46.63	46.225	46.2355
(repeated)	32.8	47.01	46.8101	46.8247
(repeated)	56.4	49.19	48.743	48.7713
(repeated)	94	51.18	50.5861	50.6275
(repeated)	98.2	51.59	50.7447	50.7873
(repeated)	123	52.22	51.5647	51.6132
(repeated)	259	54.71	54.3061	54.3746
GCCGGC/CGGCCG	8.73	52.34	51.4748	51.3017
(repeated)	20.8	54.73	54.3937	54.2876
(repeated)	27	55.73	55.2811	55.1956
(repeated)	47.5	57.5	57.2192	57.1791
(repeated)	81.2	59.67	59.0801	59.084
(repeated)	99.4	59.63	59.7875	59.8083
(repeated)	110	60.26	60.143	60.1723
(repeated)	124	61.29	60.5643	60.6038
(repeated)	204	63.03	62.3267	62.4087
(repeated)	601	66.07	66.2163	66.394
GAGCUC/CUCGAG	8.22	31.44	32.27	32.2219
(repeated)	14.8	33.8	34.153	34.1063
(repeated)	24.7	35.06	35.812	35.7665
(repeated)	44.6	37.41	37.7486	37.7045
(repeated)	77.5	39.28	39.5814	39.5387
(repeated)	127	41.25	41.2381	41.1967
(repeated)	195	42.51	42.6907	42.6505
(repeated)	370	44.74	44.8857	44.8472
(repeated)	637	47.2	46.7715	46.7345
CCUAGG/GGAUCC	8.46	32.44	31.3843	31.558
(repeated)	9.63	32.59	31.8188	31.9873
(repeated)	11.3	32.84	32.3569	32.519
(repeated)	21.7	34.95	34.5724	34.7079
(repeated)	37.1	36.54	36.4175	36.5307
(repeated)	62.9	43.22	38.2556	38.3461
(repeated)	99	39.46	39.8523	39.9229
(repeated)	178	41.54	41.9419	41.9863
(repeated)	313	43.22	43.9788	43.9972
CCAUGG/GGUACC	8.26	28.01	27.6908	27.666
(repeated)	9.65	27.55	28.2141	28.1919

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Table S1: (continued) Sequences for data set `D-RW-71`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	15.8	29.4	29.8851	29.8712
(repeated)	30.2	32.62	32.109	32.1063
(repeated)	49.1	33.61	33.799	33.805
(repeated)	83.5	34.98	35.6669	35.6825
(repeated)	148	37.52	37.7059	37.7322
(repeated)	244	38.83	39.5092	39.5451
(repeated)	445	39.99	41.7044	41.7521
ACCGGU/UGGCCA	6.99	33.27	33.7162	33.5023
(repeated)	7.37	35.03	33.9146	33.7064
(repeated)	12.9	37.18	36.0295	35.8823
(repeated)	21.9	39.09	38.0559	37.968
(repeated)	28.9	38.59	39.1284	39.0722
(repeated)	46	40.82	40.9425	40.9405
(repeated)	74.2	43.29	42.8308	42.8857
(repeated)	110	45.38	44.4028	44.5058
(repeated)	117	42.2	44.6505	44.7611
GACGUC/CUGCAG	8.27	30.34	30.0689	30.112
(repeated)	9.24	30.94	30.4277	30.4719
(repeated)	15.8	32.3	32.1757	32.2247
(repeated)	28.7	34.45	34.1444	34.1989
(repeated)	48.9	35.72	35.9236	35.983
(repeated)	82.5	37.89	37.6899	37.7544
(repeated)	125	39.49	39.1077	39.1763
(repeated)	232	41.32	41.2419	41.3167
(repeated)	417	43.44	43.2925	43.3733
AGCGCU/UCGCGA	8.46	31.06	31.761	31.7337
(repeated)	10.8	32.68	32.6621	32.6488
(repeated)	11	31.12	32.7301	32.7178
(repeated)	14.6	32.87	33.782	33.7861
(repeated)	16.3	35.89	34.1932	34.2037
(repeated)	22.2	33.84	35.3525	35.3811
(repeated)	31.1	38.5	36.6275	36.6763
(repeated)	36.4	35.22	37.2263	37.2846
(repeated)	42.4	37.48	37.8091	37.8767
(repeated)	56.2	40.41	38.8911	38.9762
(repeated)	76.8	39.98	40.0992	40.2038
(repeated)	89.4	40.15	40.6903	40.8044
(repeated)	89.8	42	40.7077	40.8221
(repeated)	153	43.13	42.7989	42.9476
(repeated)	163	45.35	43.0492	43.2021
(repeated)	259	42.9	44.8922	45.0758
CACGUG/GUGCAC	6.68	24.88	24.4954	24.5463
(repeated)	7.14	24.29	24.7179	24.7685
(repeated)	12.3	26.41	26.5475	26.5957
(repeated)	20.9	28.2	28.3526	28.3984
(repeated)	23.8	28.9	28.7983	28.8436
(repeated)	39.3	29.66	30.5313	30.5742
(repeated)	66.6	32.34	32.3755	32.4159

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Table S1: (continued) Sequences for data set `D-RW-71`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	110	34.5	34.1508	34.1887
(repeated)	121	34.2	34.4903	34.5277
(repeated)	200	36.19	36.293	36.3279
(repeated)	557	39.86	40.0334	40.063
(repeated)	3347	37.77	46.8046	46.8241
AGAUAUCU/UCUAUAGA	7.29	23.62	23.4325	23.5263
(repeated)	12.2	24.55	24.8513	24.9076
(repeated)	14.1	25.13	25.2526	25.2982
(repeated)	20.3	26.51	26.2678	26.2862
(repeated)	24.4	26.57	26.7828	26.7874
(repeated)	41.1	28.46	28.2523	28.2172
(repeated)	62	29.83	29.4212	29.3542
(repeated)	113	31.31	31.1442	31.0297
(repeated)	200	32.9	32.8013	32.6406
ACUUAAGU/UGAAUUCA	6.46	20.79	23.1687	23.188
(repeated)	11.1	22.6	24.8652	24.8779
(repeated)	12.4	23.19	25.2147	25.226
(repeated)	18.9	24.38	26.5523	26.5582
(repeated)	22	24.94	27.0372	27.0413
(repeated)	38.1	27.13	28.8039	28.8008
(repeated)	56.8	28.05	30.1016	30.0932
(repeated)	105	29.7	32.1202	32.1036
(repeated)	187	31.79	34.0411	34.0165
ACUAUAGU/UGAUAUCA	7.54	24.91	25.5837	25.6881
(repeated)	12.8	26.8	27.0642	27.1145
(repeated)	12.9	26.84	27.0861	27.1356
(repeated)	21.8	28.73	28.5686	28.5635
(repeated)	22.7	28.56	28.6835	28.6741
(repeated)	40.2	30.38	30.3164	30.2461
(repeated)	58.7	31.41	31.4077	31.2964
(repeated)	106	33	33.1273	32.9507
(repeated)	194	34.76	34.9061	34.6613
AACUAGUU/UUGAUCAA	6.37	25.4	23.125	23.1445
(repeated)	11.3	26.85	24.9215	24.934
(repeated)	13.9	28	25.5759	25.5858
(repeated)	19.4	28.89	26.6355	26.6412
(repeated)	25.3	29.77	27.4849	27.4871
(repeated)	42.9	31.56	29.1883	29.1837
(repeated)	67	32.87	30.6416	30.631
(repeated)	122	34.39	32.6173	32.5987
(repeated)	216	36.33	34.5247	34.498

Table S2: Sequences for data set `D-RW-121`, shown are the experimental temperatures T_{exp} and corresponding predictions.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
CUGCAG/GACGUC	7.95	31.31	29.9026	29.7952
(repeated)	14.9	33.29	32.0256	31.9027
(repeated)	25.3	35.35	33.838	33.7017
(repeated)	46.5	37.29	35.9484	35.7963
(repeated)	79.2	39.06	37.8188	37.6525
(repeated)	130	41.05	39.5798	39.4
(repeated)	202	42.49	41.1629	40.9708
(repeated)	364	44.17	43.3032	43.0944
(repeated)	683	46.59	45.623	45.3958
CAGCUG/GUCGAC	6.82	27.14	29.389	29.2853
(repeated)	12.1	29.61	31.3188	31.2011
(repeated)	21.5	31.93	33.2786	33.1464
(repeated)	40.1	34.08	35.4323	35.2841
(repeated)	67.5	36.49	37.255	37.093
(repeated)	111	38.29	39.0162	38.8407
(repeated)	179	39.24	40.7271	40.5384
(repeated)	325	40.94	42.889	42.6835
(repeated)	562	43.44	44.9006	44.6792
GCGCGC/CGCGCG	9.42	48.47	50.2891	49.9835
(repeated)	11.6	50.6	50.9715	50.6883
(repeated)	15.9	51.21	52.0105	51.7618
(repeated)	21.1	51.54	52.9487	52.7311
(repeated)	25.3	52.83	53.5534	53.3561
(repeated)	26.9	53.19	53.7581	53.5677
(repeated)	46.5	55.15	55.5973	55.4691
(repeated)	79.9	57.09	57.4368	57.3714
(repeated)	119	58.44	58.8036	58.7854
(repeated)	126	58.43	59.0007	58.9893
(repeated)	129	59.59	59.0819	59.0733
(repeated)	221	60.29	60.9503	61.007
(repeated)	390	63.32	62.9445	63.0717
(repeated)	656	64.77	64.7913	64.9846
CGCGCG/GCGCGC	7.79	44.53	44.4079	44.3295
(repeated)	11	45.53	45.5764	45.5189
(repeated)	16.5	47.24	46.9604	46.928
(repeated)	17.6	46.61	47.1819	47.1534
(repeated)	25.3	48.32	48.4326	48.427
(repeated)	29.4	49.3	48.9531	48.957
(repeated)	32.8	49.39	49.3334	49.3443
(repeated)	55.8	51.15	51.1928	51.2381
(repeated)	87	53.03	52.7636	52.8383
(repeated)	96.3	54.25	53.1249	53.2064
(repeated)	137	54.73	54.3853	54.4906
(repeated)	269	57.46	56.8251	56.9771
(repeated)	505	60.09	59.1357	59.3325
GCCGGC/CGGCCG	8.38	54.69	53.801	53.3108
(repeated)	19.6	57	56.6703	56.3492

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Table S2: (continued) Sequences for data set `D-RW-121`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	26.5	58.02	57.701	57.4414
(repeated)	45.8	59.91	59.5872	59.4413
(repeated)	76.7	61.94	61.3846	61.3482
(repeated)	78.6	61.74	61.4703	61.4393
(repeated)	120	63.29	62.9606	63.0214
(repeated)	122	63.57	63.0191	63.0835
(repeated)	213	64.89	65.0029	65.191
(repeated)	365	66.81	66.9426	67.2532
(repeated)	607	69.12	68.7949	69.2238
GCAUGC/CGUACG	8.68	31.87	31.6504	31.7808
(repeated)	15.1	33.7	33.4311	33.5733
(repeated)	25.6	35.91	35.1484	35.3021
(repeated)	46.2	37.7	37.0919	37.2587
(repeated)	78.9	39.45	38.8751	39.054
(repeated)	128	41.24	40.5048	40.695
(repeated)	214	43.02	42.2547	42.4571
(repeated)	386	44.81	44.2873	44.5041
(repeated)	649	46.64	46.0997	46.3293
CGGCCG/GCCGGC	7.65	47.73	48.365	47.9105
(repeated)	12.8	48.76	50.1582	49.7815
(repeated)	15.8	50.42	50.8974	50.5531
(repeated)	35.5	53.75	53.7714	53.5543
(repeated)	60.2	55.38	55.6741	55.5426
(repeated)	83.9	56.51	56.8814	56.8047
(repeated)	95.1	57.47	57.3394	57.2836
(repeated)	105	58.25	57.7023	57.6631
(repeated)	166	59.24	59.391	59.4297
(repeated)	306	61.53	61.6731	61.8183
(repeated)	522	64.01	63.6917	63.9323
GAGCUC/CUCGAG	8.81	34.78	35.3111	35.1671
(repeated)	15.6	36.2	37.1041	36.9729
(repeated)	26.6	37.85	38.7976	38.6787
(repeated)	48.8	40.36	40.746	40.6413
(repeated)	83.8	42.19	42.5027	42.411
(repeated)	139	44	44.1647	44.0855
(repeated)	216	45.04	45.6267	45.5586
(repeated)	391	47.38	47.6164	47.5635
(repeated)	692	50.21	49.5541	49.5162
ACCGGU/UGGCCA	6.54	36.31	36.1982	35.6903
(repeated)	8.36	36.84	37.172	36.7252
(repeated)	14.3	39.88	39.3225	39.0123
(repeated)	24.2	42.48	41.4593	41.2868
(repeated)	25.8	41.18	41.7214	41.5658
(repeated)	48.1	44.04	44.2938	44.307
(repeated)	81.2	46.91	46.489	46.6484
(repeated)	97.3	44.57	47.2543	47.4653
(repeated)	139	50.04	48.7743	49.0884
CCAUGG/GGUACC	7.23	28.39	28.4673	28.3657

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Table S2: (continued) Sequences for data set `D-RW-121`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	12.7	30.38	30.3838	30.3103
(repeated)	21.8	31.88	32.2448	32.199
(repeated)	40.8	34.01	34.4324	34.4195
(repeated)	69.4	35.99	36.3112	36.327
(repeated)	119	38.15	38.242	38.2876
(repeated)	190	38.58	39.937	40.0091
(repeated)	323	40.08	41.8817	41.9846
(repeated)	577	43.98	44.0359	44.1733
CCUAGG/GGAUCC	6.32	34.03	32.5382	32.935
(repeated)	7.51	34.83	33.142	33.5287
(repeated)	10.7	35.59	34.3887	34.754
(repeated)	21.8	37.49	36.9258	37.2473
(repeated)	35.7	39.48	38.7089	38.9992
(repeated)	61.4	40.99	40.6931	40.9481
(repeated)	99.4	41.26	42.4771	42.7001
(repeated)	179	44.37	44.6832	44.866
(repeated)	317	46.57	46.8563	46.999
CACGUG/GUGCAC	5.71	26.53	26.2393	26.3969
(repeated)	6.15	26.62	26.4882	26.6445
(repeated)	12	28.87	28.7479	28.8931
(repeated)	20.5	30.65	30.5829	30.7189
(repeated)	24.2	31.3	31.156	31.2891
(repeated)	40.5	33.02	32.9485	33.0725
(repeated)	68.4	34.81	34.7946	34.909
(repeated)	105	37.55	36.3209	36.4274
(repeated)	109	36.45	36.4548	36.5606
(repeated)	230	39.28	39.153	39.2444
(repeated)	325	39.74	40.4183	40.5029
AGCGCU/UCGCGA	9.78	35.6	35.9696	36.0558
(repeated)	10.4	35.09	36.2061	36.2992
(repeated)	16.7	38.33	38.0401	38.188
(repeated)	28.4	40.64	40.1223	40.3333
(repeated)	33.5	40.09	40.7756	41.0066
(repeated)	54.5	43.91	42.7167	43.0074
(repeated)	94.5	47.53	44.9412	45.3013
(repeated)	146	45.69	46.7216	47.138
(repeated)	158	47.39	47.047	47.4738
GACGUC/CUGCAG	8.28	32.56	32.8592	32.9275
(repeated)	9.24	33.6	33.2033	33.2748
(repeated)	16.5	35.14	35.0347	35.1236
(repeated)	27.9	36.59	36.7129	36.8178
(repeated)	49	38.74	38.5327	38.6551
(repeated)	83.4	40.74	40.2708	40.4102
(repeated)	129	42.13	41.7108	41.8644
(repeated)	232	44.14	43.6696	43.8427
(repeated)	426	46.02	45.7236	45.9174
AGAUAUCU/UCUAUAGA	8.06	26.02	26.5141	26.6845
(repeated)	14.2	28.43	28.0834	28.174

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Table S2: (continued) Sequences for data set `D-RW-121`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	15.1	28.07	28.2547	28.3366
(repeated)	22.2	29.6	29.3333	29.3598
(repeated)	27.5	30.51	29.9358	29.9313
(repeated)	43.7	31.6	31.2476	31.175
(repeated)	64	32.6	32.3367	32.2071
(repeated)	125	34.82	34.2666	34.0352
(repeated)	220	35.77	35.9154	35.5961
ACUUAAGU/UGAAUUCA	7.43	24.7	26.834	26.8405
(repeated)	12.9	26.08	28.4013	28.4059
(repeated)	13.7	26.4	28.5733	28.5776
(repeated)	21.8	27.87	29.9072	29.9098
(repeated)	24.5	28.05	30.2444	30.2466
(repeated)	42.7	30.12	31.8588	31.859
(repeated)	60.4	31.42	32.8754	32.8742
(repeated)	111	32.5	34.6757	34.6723
(repeated)	201	34.37	36.4529	36.4471
ACUAUAGU/UGAUAUCA	5.69	27.39	27.8273	28.1055
(repeated)	9.94	29.04	29.4788	29.6316
(repeated)	15.4	30.5	30.7877	30.8401
(repeated)	16.8	30.38	31.0491	31.0815
(repeated)	27.2	32.16	32.5053	32.4249
(repeated)	44.7	33.72	34.0212	33.8224
(repeated)	84.7	35.63	35.9938	35.6394
(repeated)	152	37.56	37.821	37.3208
(repeated)	249	39.29	39.3801	38.7543
AACUAGUU/UUGAUCAA	6.71	28.5	26.5462	26.553
(repeated)	11.6	29.99	28.0983	28.1032
(repeated)	17.9	31.69	29.3397	29.3431
(repeated)	19.4	31.41	29.5712	29.5742
(repeated)	31.1	33.32	30.9355	30.9368
(repeated)	50	34.98	32.3206	32.3202
(repeated)	73.8	36.11	33.4658	33.4639
(repeated)	128	37.67	35.1004	35.0964

Table S3: Sequences for data set `D-RW-221`, shown are the experimental temperatures T_{exp} and corresponding predictions.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
GAGCUC/CUCGAG	8.82	36.83	37.3503	37.2835
(repeated)	15.7	38.61	39.2002	39.136
(repeated)	26.9	40.14	40.9476	40.886
(repeated)	48.1	42.44	42.8557	42.7968
(repeated)	82.2	44.57	44.6357	44.5794
(repeated)	134	46.58	46.2766	46.2227
(repeated)	214	47.43	47.8644	47.8129
(repeated)	380	49.67	49.8337	49.7852
(repeated)	676	51.62	51.8336	51.7882
ACCGGU/UGGCCA	6.22	37.77	38.8995	38.522
(repeated)	6.68	39.34	39.1805	38.8195
(repeated)	8.78	40.81	40.262	39.9644
(repeated)	12.8	42.04	41.7657	41.5572
(repeated)	22.1	42.72	43.9699	43.8936
(repeated)	25.2	43.18	44.5043	44.4604
(repeated)	44.6	49.13	46.8496	46.9491
(repeated)	74.3	48.68	48.9759	49.2072
(repeated)	129	50.37	51.3063	51.6843
CCAUGG/GGUACC	7.18	32.02	31.8889	31.814
(repeated)	8.29	32.67	32.3693	32.3006
(repeated)	14.9	34.11	34.3441	34.3014
(repeated)	29.6	36.66	36.6888	36.6774
(repeated)	49.8	38.55	38.4898	38.5028
(repeated)	83	40.37	40.2787	40.3161
(repeated)	137	41.35	42.0538	42.1158
(repeated)	240	42.97	44.0637	44.1538
(repeated)	428	44.81	46.1645	46.2844
CCUAGG/GGAUCC	6.98	36.1	35.2902	35.5521
(repeated)	8.98	37.18	36.1566	36.4103
(repeated)	11.7	37.84	37.0717	37.3167
(repeated)	21.3	39.74	39.1639	39.3888
(repeated)	37.4	41.74	41.1558	41.3613
(repeated)	63.1	43.64	43.0294	43.2164
(repeated)	109	44.84	45.0114	45.1786
(repeated)	201	46.79	47.26	47.4044
(repeated)	348	48.66	49.3041	49.4275
CACGUG/GUGCAC	7.06	28.97	29.2673	29.3739
(repeated)	7.13	28.98	29.2999	29.4063
(repeated)	13.7	31.59	31.4729	31.5683
(repeated)	23	33.52	33.2191	33.3056
(repeated)	23.7	33.32	33.3207	33.4067
(repeated)	40.4	35.56	35.1406	35.2172
(repeated)	72.6	38.27	37.1657	37.2316
(repeated)	109	38.57	38.5854	38.6438
(repeated)	119	39.3	38.8937	38.9505
(repeated)	190	40.02	40.5478	40.5957
AGCGCU/UCGCGA	9.73	37.96	38.7223	38.7597

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Table S3: (continued) Sequences for data set `D-RW-221`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	10.3	37.79	38.9326	38.9757
(repeated)	17.1	41.12	40.8176	40.9125
(repeated)	29.7	45.15	42.8965	43.0492
(repeated)	30.9	42.92	43.0467	43.2036
(repeated)	53.7	46.1	45.1575	45.3741
(repeated)	93.6	49.02	47.3083	47.5864
(repeated)	160	50.44	49.4114	49.7505
(repeated)	161	47.02	49.436	49.7758
GACGUC/CUGCAG	7.31	33.82	34.0438	34.0998
(repeated)	10.1	35.1	35.1075	35.1683
(repeated)	17.3	37.51	36.8945	36.9635
(repeated)	28.3	38.79	38.547	38.6237
(repeated)	49.5	40.49	40.4458	40.5314
(repeated)	83.3	43.01	42.2342	42.3284
(repeated)	120	43.48	43.5008	43.6011
(repeated)	227	46.01	45.7372	45.8484
(repeated)	420	48.04	47.926	48.0479
CUGCAG/GACGUC	8.36	33.04	32.7716	32.7317
(repeated)	9.34	33.53	33.128	33.0853
(repeated)	15.8	35.59	34.8298	34.7736
(repeated)	26.4	37.35	36.5099	36.4402
(repeated)	30.2	37.44	36.953	36.8798
(repeated)	47	39.41	38.4196	38.3345
(repeated)	79.6	41.39	40.1847	40.0852
(repeated)	118	42.22	41.5168	41.4062
(repeated)	130	43	41.8462	41.7329
(repeated)	208	44.61	43.4548	43.328
(repeated)	379	46.37	45.5323	45.3879
(repeated)	655	48.53	47.4505	47.2897
CAGCUG/GUCGAC	7.75	30.55	32.5284	32.4905
(repeated)	13.5	33.26	34.3185	34.2664
(repeated)	22.8	35.17	36.0282	35.9624
(repeated)	39.3	36.43	37.8247	37.7444
(repeated)	68.2	38.85	39.6648	39.5695
(repeated)	111	41.13	41.3091	41.2002
(repeated)	191	41.33	43.1617	43.0374
(repeated)	328	43.85	45.0294	44.8893
(repeated)	572	45.18	46.9733	46.8166
GCGCGC/CGCGCG	8.78	51.64	51.9164	51.6843
(repeated)	19.5	53.94	54.575	54.4096
(repeated)	25.6	54.69	55.4918	55.3497
(repeated)	26.6	54.4	55.6213	55.4825
(repeated)	43.3	57.23	57.2767	57.1804
(repeated)	80.6	59.33	59.4121	59.3712
(repeated)	102	59.71	60.2286	60.2091
(repeated)	127	61.25	60.9923	60.9929
(repeated)	136	61.08	61.2316	61.2385
(repeated)	209	62.24	62.7409	62.7879

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Table S3: (continued) Sequences for data set `D-RW-221`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	379	65.25	64.8544	64.958
(repeated)	633	66.42	66.6971	66.8508
CGCGCG/GCGCGC	8.53	46.64	46.565	46.4851
(repeated)	16.8	47.71	48.8311	48.7829
(repeated)	17.2	49.04	48.9103	48.8633
(repeated)	23.2	49.83	49.9215	49.8888
(repeated)	30.4	50.9	50.8403	50.8207
(repeated)	52.1	53.5	52.6873	52.6943
(repeated)	89.9	55.29	54.5793	54.6137
(repeated)	91.2	54.71	54.6294	54.6645
(repeated)	110	55.44	55.2847	55.3294
(repeated)	147	56.27	56.3036	56.3634
(repeated)	254	58.75	58.2428	58.3314
GCCGGC/CGGCCG	8.8	56.93	56.3086	56.0682
(repeated)	9.86	57.33	56.6971	56.4751
(repeated)	13.7	57.13	57.8257	57.6576
(repeated)	15.4	58.01	58.229	58.0801
(repeated)	20.6	59.34	59.2361	59.1358
(repeated)	25.6	60.89	59.9925	59.9287
(repeated)	27.1	60.29	60.1912	60.1371
(repeated)	47	62.12	62.1254	62.1659
(repeated)	80	64.19	64.0152	64.1492
(repeated)	120	65.89	65.4702	65.677
GCAUGC/CGUACG	8.91	33.9	34.2655	34.3593
(repeated)	15.8	36.56	36.1285	36.2294
(repeated)	27.6	38.32	37.9645	38.0726
(repeated)	48.8	40.19	39.8631	39.9785
(repeated)	80.8	42.03	41.5623	41.6844
(repeated)	135	43.98	43.311	43.4401
(repeated)	228	45.55	45.1166	45.253
(repeated)	407	47.38	47.1372	47.2818
(repeated)	692	49.43	49.0107	49.163
CGGCCG/GCCGGC	8.46	50.29	50.9152	50.6618
(repeated)	9.86	50.88	51.441	51.2064
(repeated)	11.1	51.26	51.849	51.629
(repeated)	17.4	53.1	53.4064	53.2426
(repeated)	22.8	53.53	54.3501	54.2205
(repeated)	38.6	55.82	56.204	56.1424
(repeated)	63.5	58.43	57.9762	57.9803
(repeated)	83.7	59	58.9677	59.009
(repeated)	102	59.6	59.6813	59.7493
(repeated)	310	64.85	63.7503	63.9736
AACUAGUU/UUGAUCAA	6.6	31.13	29.3118	29.3496
(repeated)	11.4	33.11	31.0008	31.0266
(repeated)	16.8	34.25	32.2106	32.2277
(repeated)	19.3	34.72	32.6457	32.6597
(repeated)	29.2	35.94	33.952	33.9565
(repeated)	48.7	37.68	35.5811	35.5737

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Table S3: (continued) Sequences for data set `D-RW-221`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	66.7	38.77	36.5915	36.5767
(repeated)	120	40.59	38.4959	38.4669
(repeated)	209	42.2	40.3167	40.274
AGAUAUCU/UCUAUAGA	7.86	29.4	29.9704	30.0746
(repeated)	13.7	31.31	31.5338	31.5867
(repeated)	15.5	31.71	31.8834	31.9247
(repeated)	22.1	33.14	32.8924	32.9002
(repeated)	27.7	33.61	33.5383	33.5245
(repeated)	45.1	35.61	34.9416	34.8807
(repeated)	74.3	36.26	36.3922	36.2821
(repeated)	133	38.62	38.1013	37.9327
(repeated)	221	40.41	39.6075	39.3868
ACUUAAGU/UGAAUUCA	7.32	27.36	29.6303	29.6659
(repeated)	12.6	29.35	31.3121	31.3357
(repeated)	14.3	29.63	31.7067	31.7275
(repeated)	21.2	31.26	32.941	32.9528
(repeated)	25.2	31.51	33.486	33.4939
(repeated)	42.7	33.29	35.1607	35.1564
(repeated)	67.3	34.5	36.6204	36.6053
(repeated)	123	36.48	38.5765	38.5468
(repeated)	211	38.12	40.3481	40.3052
ACUAUAGU/UGAUAUCA	6.84	30.65	30.9974	31.1339
(repeated)	12.3	32.63	32.7409	32.7913
(repeated)	12.7	32.55	32.8365	32.8822
(repeated)	20.6	34.3	34.2896	34.2628
(repeated)	23.5	34.61	34.6877	34.6409
(repeated)	39.3	36.01	36.2517	36.126
(repeated)	65.2	37.41	37.8071	37.6021
(repeated)	120	39.29	39.7023	39.3997
(repeated)	205	40.92	41.3851	40.9949

Table S4: Sequences for data set `D-RW-621`, shown are the experimental temperatures T_{exp} and corresponding predictions.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
GAGCUC/CUCGAG	8.21	38.93	39.7421	39.5726
(repeated)	15.2	41.1	41.782	41.6366
(repeated)	26.8	43.04	43.6838	43.5612
(repeated)	46.7	45.06	45.5686	45.4689
(repeated)	81.3	47.34	47.4727	47.3964
(repeated)	135	48.99	49.2344	49.18
(repeated)	207	50.17	50.7345	50.6989
(repeated)	387	52.44	52.9556	52.9483
(repeated)	681	54.65	54.9881	55.0069
CCUAGG/GGAUCC	6.27	38.18	37.4622	37.6915
(repeated)	6.89	38.56	37.7984	38.0296
(repeated)	13.1	41.01	40.109	40.3528
(repeated)	17.7	41.97	41.2032	41.4529
(repeated)	20.8	42.12	41.793	42.046
(repeated)	35.5	44.24	43.7628	44.0267
(repeated)	59.7	46.54	45.702	45.9767
(repeated)	67.5	46.48	46.1635	46.4409
(repeated)	86.2	47.43	47.0867	47.3693
(repeated)	101	45.58	47.6877	47.9737
CCAUGG/GGUACC	6.3	34.53	34.804	34.7136
(repeated)	7.34	35.45	35.2967	35.2132
(repeated)	14	38.04	37.3962	37.3423
(repeated)	24.7	39.75	39.266	39.2388
(repeated)	42.4	41.51	41.0666	41.0654
(repeated)	73.9	43.85	42.9397	42.9659
(repeated)	120	42.88	44.5924	44.6431
(repeated)	213	45.36	46.5712	46.6514
(repeated)	390	47.47	48.6838	48.7961
ACCGGU/UGGCCA	5.86	38.34	41.1806	40.7197
(repeated)	6.53	39.49	41.5855	41.1488
(repeated)	7.55	44.06	42.13	41.726
(repeated)	12.7	46.46	44.0966	43.8116
(repeated)	24.5	46.71	46.6167	46.4866
(repeated)	31.5	47.02	47.5912	47.5217
(repeated)	41.2	48.84	48.6387	48.6347
(repeated)	65.9	52.13	50.4881	50.601
(repeated)	96.2	49.92	51.9931	52.2022
(repeated)	99.6	54.14	52.1319	52.35
(repeated)	117	49.93	52.7773	53.0369
GACGUC/CUGCAG	8.2	36.57	37.1818	37.2046
(repeated)	11	38.33	38.106	38.144
(repeated)	14.3	39.27	38.9361	38.9878
(repeated)	26.8	41.13	40.9415	41.0267
(repeated)	45.8	44.02	42.6728	42.7874
(repeated)	75.4	45.22	44.3007	44.443
(repeated)	222	48.85	47.8851	48.0897
(repeated)	385	50.4	49.744	49.9813

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Table S4: (continued) Sequences for data set `D-RW-621`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
CACGUG/GUGCAC	5.35	30.96	31.7266	31.9051
(repeated)	5.49	31.21	31.8057	31.9836
(repeated)	10.3	33.81	33.7451	33.9089
(repeated)	18.2	36.59	35.5212	35.6718
(repeated)	20.3	35.68	35.8642	36.0123
(repeated)	34.5	37.7	37.5411	37.6767
(repeated)	59.7	40.37	39.2943	39.4166
(repeated)	93.8	42.65	40.7537	40.8649
(repeated)	98.9	40.8	40.9257	41.0355
(repeated)	170	42.32	42.6954	42.7915
(repeated)	304	44.04	44.6166	44.6976
(repeated)	482	45.21	46.1568	46.2257
AGCGCU/UCGCGA	5.09	39.31	38.9348	39.0553
(repeated)	8.05	38.52	40.697	40.8485
(repeated)	12.2	42.95	42.3125	42.4928
(repeated)	21	43.5	44.448	44.6668
(repeated)	21.9	48.86	44.6142	44.8361
(repeated)	33.3	46.44	46.2837	46.536
(repeated)	57.7	50.51	48.5003	48.7936
(repeated)	96.1	47.88	50.5851	50.9174
(repeated)	104	52.69	50.9104	51.2488
CUGCAG/GACGUC	7.91	35.6	35.3061	35.2525
(repeated)	8.89	36.18	35.6844	35.6259
(repeated)	11.3	37.4	36.4642	36.3957
(repeated)	13	37.38	36.9216	36.8472
(repeated)	17.4	38.23	37.8774	37.7906
(repeated)	22.6	39.9	38.7397	38.6417
(repeated)	23.3	39.18	38.8406	38.7413
(repeated)	40.4	41.66	40.6727	40.5492
(repeated)	69.9	44.96	42.5191	42.3711
(repeated)	85.1	43.44	43.187	43.0301
(repeated)	104	44.56	43.8708	43.7047
(repeated)	119	45.94	44.3319	44.1595
(repeated)	200	46.79	46.121	45.9243
(repeated)	348	49.07	48.0521	47.8289
(repeated)	631	51.66	50.1531	49.9007
GCGCGC/CGCGCG	8.73	54.09	54.3045	53.9973
(repeated)	12	53.96	55.3743	55.1109
(repeated)	16.7	55.9	56.4932	56.2757
(repeated)	18.9	56.5	56.9141	56.714
(repeated)	29	57.52	58.3786	58.2394
(repeated)	50.4	59.54	60.2885	60.2296
(repeated)	79.6	62.02	61.8844	61.8934
(repeated)	86.8	62.33	62.1886	62.2105
(repeated)	103	61.92	62.7912	62.839
(repeated)	129	63.88	63.5871	63.6692
(repeated)	138	62.84	63.8263	63.9187
(repeated)	206	64.6	65.2544	65.4088

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Table S4: (continued) Sequences for data set `D-RW-621`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
CAGCUG/GUCGAC	6.4	32.3	34.6224	34.5775
(repeated)	11.6	34.41	36.5496	36.48
(repeated)	19.2	36.74	38.2015	38.1105
(repeated)	34.2	38.86	40.1158	39.9997
(repeated)	60.5	41.06	42.0305	41.8891
(repeated)	96.7	42.6	43.6224	43.4596
(repeated)	160	43.58	45.3496	45.1634
(repeated)	302	45.32	47.5556	47.3392
(repeated)	487	47.43	49.2352	48.9956
GCAUGC/CGUACG	8.54	37.26	37.5152	37.6791
(repeated)	15.1	39.25	39.3097	39.4821
(repeated)	26.5	41.67	41.1011	41.282
(repeated)	43.1	43.12	42.6669	42.8553
(repeated)	74.4	44.79	44.443	44.64
(repeated)	136	47.35	46.4289	46.6356
(repeated)	231	48.63	48.1935	48.4091
(repeated)	410	50.43	50.1268	50.352
(repeated)	696	52.18	51.9307	52.165
GCCGGC/CGGCCG	8.74	58.72	58.591	58.2434
(repeated)	10.6	59.8	59.2556	58.9591
(repeated)	12.1	60.66	59.7131	59.4518
(repeated)	13.8	60.9	60.1688	59.9426
(repeated)	18.7	60.81	61.2267	61.0827
(repeated)	24.5	63	62.1729	62.1029
(repeated)	24.6	62.4	62.1872	62.1183
(repeated)	43.2	64.31	64.1771	64.2651
(repeated)	72.4	66.64	66.0226	66.2581
(repeated)	119	68.25	67.8179	68.1983
CGCGCG/GCGCGC	7.59	48.67	48.432	48.2969
(repeated)	8.4	47.74	48.7751	48.6464
(repeated)	15	51.06	50.7509	50.6596
(repeated)	21.1	51.87	51.9251	51.8562
(repeated)	29.5	53.1	53.0865	53.0401
(repeated)	48.8	55.21	54.8467	54.8345
(repeated)	82.1	56.99	56.686	56.7099
(repeated)	103	57.64	57.4943	57.5342
(repeated)	130	59.19	58.3282	58.3847
(repeated)	176	59.21	59.4196	59.498
(repeated)	303	61.93	61.3949	61.5133
(repeated)	677	65.71	64.3615	64.5408
CGGCCG/GCCGGC	8.76	52.26	53.2536	52.8117
(repeated)	10.2	52.1	53.784	53.3702
(repeated)	17.6	55.32	55.6994	55.3881
(repeated)	21.5	55.04	56.4078	56.1348
(repeated)	35.5	57.87	58.1962	58.0205
(repeated)	57.3	60.57	59.9218	59.841
(repeated)	82.9	61.11	61.2653	61.2592
(repeated)	96.5	62.12	61.821	61.846

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Table S4: (continued) Sequences for data set `D-RW-621`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
(repeated)	111	62.31	62.3348	62.3886
(repeated)	278	66.1	65.7437	65.991
(repeated)	503	68.16	67.9825	68.3592
AACUAGUU/UUGAUCAA	5.59	34.52	31.9433	31.9808
(repeated)	7.98	34.92	33.1001	33.1288
(repeated)	10.9	36.26	34.1208	34.1416
(repeated)	19.8	38.68	36.0937	36.0992
(repeated)	35.5	40.11	38.048	38.0382
(repeated)	51.9	41.76	39.3326	39.3126
(repeated)	97.5	43.62	41.4889	41.4516
(repeated)	179	45.81	43.5949	43.5405
AGAUAUCU/UCUAUAGA	7.61	33.43	33.9071	34.1109
(repeated)	13.6	35.52	35.5748	35.6938
(repeated)	15.2	35.69	35.8963	35.9989
(repeated)	22.6	37.46	37.0485	37.0919
(repeated)	27.4	37.53	37.6111	37.6254
(repeated)	45.6	39.23	39.1088	39.0452
(repeated)	73.1	40.59	40.5093	40.3722
(repeated)	134	42.52	42.3263	42.093
(repeated)	228	44.51	43.9373	43.6178
ACUUAAGU/UGAAUUCA	5.46	30.04	31.8671	31.9052
(repeated)	9.52	31.91	33.6769	33.7011
(repeated)	10.7	32.28	34.06	34.0813
(repeated)	16.5	33.67	35.4884	35.4986
(repeated)	19	34.09	35.9565	35.9631
(repeated)	32.8	35.84	37.7818	37.7741
(repeated)	44.1	36.62	38.7804	38.7648
(repeated)	79.4	38.42	40.7834	40.7517
(repeated)	142	40.37	42.7889	42.741
ACUAUAGU/UGAUAUCA	7.24	34.68	35.2065	35.311
(repeated)	13	36.87	36.9216	36.9259
(repeated)	13.7	36.7	37.0762	37.0714
(repeated)	21.9	38.38	38.4658	38.3791
(repeated)	24.5	38.77	38.8	38.6935
(repeated)	43.2	40.32	40.5006	40.2926
(repeated)	70.4	41.67	41.9799	41.6827
(repeated)	128	43.49	43.8098	43.4013
(repeated)	218	44.96	45.4576	44.9479

Table S5: Sequences for data set `D-RW-EXT1021`, shown are the experimental temperatures T_{exp} and corresponding predictions.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
GCGC/CGCG	100	26.6	28.5928	27.5261
GGCC/CCGG	100	34.3	35.53	35.0296
CGCG/GCGC	100	19.3	18.9562	18.4545
CCGG/GGCC	100	27.2	26.6713	26.7477
GCUCG/CGAGC	200	37.2	37.1687	36.5198
AGCGA/UCGCU	200	30.2	29.8213	31.3504
CACUG/GUGAC	200	16.4	21.8651	21.3533
ACGCA/UGCGU	200	29.4	27.9682	29.9596
CACAG/GUGUC	200	24.5	21.8651	21.3533
GCACG/CGUGC	200	37.5	36.0165	35.4786
GCUAGC/CGAUCG	100	49.3	48.4767	48.3087
GGCGCC/CCGCGG	100	65.2	66.7074	66.6795
GCCGGC/CGGCCG	7.63	59.05	57.7183	58.2388
(repeated)	15.2	60.57	60.0791	60.4583
(repeated)	21.8	62.09	61.3278	61.6315
(repeated)	38.2	64.23	63.2889	63.4728
(repeated)	65.9	66.34	65.2175	65.2824
(repeated)	100	67.2	66.7074	66.6795
(repeated)	104	67.16	66.8482	66.8114
(repeated)	109	68.44	67.017	66.9696
(repeated)	548	73.04	72.9234	72.4998
GAGCUG/CUCGAC	200	45.5	47.3519	47.0517
GUGGUG/CACCAC	200	47.4	47.3078	47.1509
CAGCUG/GUCGAC	100	43.1	45.9993	45.8677
GCAACG/CGUUGC	200	42.6	42.1956	41.8461
GAGGAG/CUCCUC	200	50.9	48.2018	47.9586
UGCGCA/ACGCGU	100	53.1	51.3444	51.7536
GCGCCG/CGCGGC	200	65.2	62.6582	62.6288
GGCGCG/CCGCGC	200	61.6	62.6582	62.6288
UCCGGA/AGGCCU	100	50.1	52.5997	53.047
GAGCUC/CUCGAG	100	48.7	48.3965	48.0058
GUCGAC/CAGCUG	100	45.3	44.7606	44.2033
CCGCGG/GGCGCC	100	59.8	62.6573	62.625
GCUACG/CGAUGC	200	45	44.2186	43.8935
GCAUGC/CGUACG	100	45.7	47.8296	47.4572
CGCGCG/GCGCGC	100	57.8	58.249	58.2379
UGAUCA/ACUAGU	100	32.6	29.4285	29.7146
AUGCAU/UACGUA	100	30.1	29.4305	29.8315
GCCGCG/CGGCGC	200	63.9	62.6582	62.6288
GGUACC/CCAUGG	100	46.6	49.1777	49.2223
AGCGCU/UCGCGA	100	52	51.5402	51.6492
CCUAGG/GGAUCC	100	50	48.01	48.1395
GCGCGG/CGCGCC	200	61.9	62.6582	62.6288
GCGGCG/CGCCGC	200	61.8	62.6582	62.6288
CCAUGG/GGUACC	100	46.4	47.3012	47.263
GGAUCC/CCUAGG	100	47.6	49.3094	49.108
UCGCGA/AGCGCU	100	44.6	47.6796	48.1835

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Table S5: (continued) Sequences for data set `D-RW-EXT1021`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
CGUACG/GCAUGC	100	34.6	39.7809	39.2571
GUGCAG/CACGUC	200	46	46.8513	46.601
AGGCCU/UCCGGA	100	55.3	56.7416	56.4945
CGGCCG/GCCGGC	100	63.2	62.6573	62.625
CUGCAG/GACGUC	100	45.3	45.9993	45.8677
GCGCGC/CGCGCG	8.16	54.33	53.8096	54.2483
(repeated)	11.6	54.54	55.0125	55.3894
(repeated)	19.1	56.64	56.7332	57.0208
(repeated)	23.7	57.54	57.4834	57.7318
(repeated)	39.8	59.28	59.2995	59.4523
(repeated)	69.9	61.75	61.2954	61.342
(repeated)	99.2	62.4	62.5481	62.5274
(repeated)	100	62.1	62.577	62.5547
(repeated)	116	63.64	63.111	63.0599
(repeated)	126	63.06	63.4093	63.3421
(repeated)	180	64.23	64.7019	64.5644
(repeated)	334	66.58	66.966	66.7042
(repeated)	589	68.65	69.0705	68.6918
AGAGAG/UCUCUC	200	40.7	38.8813	38.9511
CACGUG/GUGCAC	100	42.8	41.7318	41.5356
GUGUCG/CACAGC	200	43.7	43.4231	43.0006
ACCGGU/UGGCCA	100	53.9	52.2386	52.4996
CAUGCG/GUACGC	200	42.9	42.3541	42.0124
UGGCCA/ACCGGU	100	55.3	56.9177	56.9946
GCGUCG/CGCAGC	200	53.7	51.3612	51.2726
UCUAGA/AGAUCU	100	31	31.5636	31.6804
GAGAGA/CUCUCU	200	40.6	40.3351	40.0932
GCAUCG/CGUAGC	200	44.1	43.8798	43.3642
GACGUC/CUGCAG	100	46.2	44.7606	44.2033
UCAUGA/AGUACU	100	27.2	29.4285	29.7146
GUGCAC/CACGUG	100	47.7	47.54	47.2096
GCUGAG/CGACUC	200	46.2	47.3519	47.0517
AGUCUGA/UCAGACU	200	45.7	48.4342	48.7566
GUCACUG/CAGUGAC	200	51.1	51.6777	51.5786
GACUCAG/CUGAGUC	200	52	51.9033	51.7863
ACUGUCA/UGACAGU	200	48.2	48.0176	48.4217
UAAGGUA/AUUCCAU	200	42.2	38.3085	38.6139
GAGUGAG/CUCACUC	200	53.7	51.9033	51.7863
AAGGAGG/UUCCUCC	200	56.2	55.859	55.809
GCAACGA/CGUUGCU	200	50.2	51.8395	51.9359
ACUUAAGU/UGAAUUCA	100	40.3	41.5212	41.9464
GUCUAGAC/CAGAUCUG	100	56.2	55.4078	55.819
GAGAGAGA/CUCUCUCU	200	57.6	58.6046	58.8295
GAACGUUC/CUUGCAAG	100	52.3	52.0902	52.0018
UUCCGGAA/AAGGCCUU	100	62.4	59.3026	59.4873
CUCGCACA/GAGCGUGU	200	64.9	64.6784	64.7043
UCCUUGCA/AGGAACGU	200	60.7	63.0178	62.8458
UAGAUCUA/AUCUAGAU	100	45.3	44.449	44.6671

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Table S5: (continued) Sequences for data set `D-RW-EXT1021`.

Sequence	C_t (μM)	T_{exp} (°C)	T_{FIF} (°C)	T_{VIF} (°C)
AAUGCAUU/UUACGUAA	100	45	40.9797	41.2457
AUGCGCAU/UACGCGUA	100	60.3	58.3874	58.5584
AGAGAGAG/UCUCUCUC	200	59.6	58.3909	58.3981
UCCGCGCA/AGGCGCGU	200	73.2	74.1671	73.6708
GUGAUCAC/CACUAGUG	100	54.4	55.2971	55.4958
GCCAUGGC/CGGUACCG	100	71.4	72.4748	72.9005
GGCUUCAA/CCGAAGUU	200	59.1	59.0896	59.0772
GAGAUCUC/CUCUAGAG	100	56.5	55.423	55.6083
AACUAGUU/UUGAUCAA	100	45.7	41.5212	41.9464
AGUUAACU/UCAAUUGA	100	41.1	41.5212	41.9464
GAUGCAUC/CUACGUAG	100	57.2	55.2588	55.4971
GCUGCGAC/CGACGCUG	200	67.9	69.4184	69.7029
AUCUAGAU/UAGAUCUA	100	45.1	44.1905	44.2207
ACCUUUGC/UGGAAACG	200	56.3	59.0355	58.8537
AUGUACAU/UACAUGUA	100	41.7	43.2471	43.3738
AGAUAUCU/UCUAUAGA	100	41.4	44.1905	44.2207
AGUAUACU/UCAUAUGA	100	44.1	44.004	44.218
UGACCUCA/ACUGGAGU	200	64.6	62.5662	62.6652
CAAAAAAG/GUUUUUUC	200	28.6	28.2945	27.9424
CGACGCAG/GCUGCGUC	200	67.1	66.3486	66.5469
GAUAUAUC/CUAUAUAG	100	39.1	40.9849	39.5829
CAUGCAUG/GUACGUAC	100	54.9	54.5502	54.7309
UUGCGCAA/AACGCGUU	100	61.2	59.1872	59.104
ACUAUAGU/UGAUAUCA	100	44	44.004	44.218
GUUCGAAC/CAAGCUUG	100	50.4	52.0902	52.0018
UAUGCAUA/AUACGUAU	100	44.4	43.8832	44.1049
UUGUACAA/AACAUGUU	100	43.6	40.8048	41.343
GUAUAUAC/CAUAUAUG	100	38.3	40.7883	39.4954
UCUAUAGA/AGAUAUCU	100	43.5	44.449	44.6671
AUACGUAU/UAUGCAUA	100	42	41.6566	41.5487
UUGGCCAA/AACCGGUU	100	65.3	63.5561	63.2145
CAAAAAAAG/GUUUUUUUC	200	33.8	34.6484	34.3693
AAGGUUGGAA/UUCCAACCUU	200	66.5	67.0434	66.71
AAAAAAAUUUUUUU/UUUUUUUAAAAAAA	100	41	43.2899	43.4966

Table S6. Validation sequences from references 1–8 for low salt concentration, shown are the experimental temperatures T_{exp} and corresponding predictions. For $T_{\text{IP-FIF}}$ and $T_{\text{IP-VIF}}$ the parameters were interpolated from the quadratic regression coefficients of tables S7 and S8, respectively. For $T_{\text{corr.}}$, the temperatures were calculated from the original parameters by Xia *et al.*[9] and afterwards the salt correction of Eq. (22) from Ref. 10 was applied. Also shown are the average difference of predicted and measured temperatures $\langle \Delta T \rangle$ and total squared difference $\chi 2$.

Sequence	C_t (μM)	[Na^+] (mM)	T_{exp} (°C)	$T_{\text{IP-FIF}}$ (°C)	$T_{\text{IP-VIF}}$ (°C)	$T_{\text{corr.}}$ (°C)
1 AGCGCU[7]	100	20	42.3	28.7336	35.477	34.7458
2 CAGGGCCCGGGCUC[1]	50	58	84	87.5036	85.9689	85.9001
3 UUUUUUUUUUUU[8]	1.4	100	12.7	15.0005	9.40242	10.0816
4 UUUUUUUUUUUU[8]	2.8	100	15.1	16.5456	11.1057	11.8194
5 UUUUUUUUUUUU[8]	4	100	16.4	17.3471	11.9902	12.7219
6 UUUUUUUUUUUU[8]	5.7	100	17.4	18.1475	12.874	13.6238
7 UUUUUUUUUUUU[8]	8	100	18	18.9176	13.725	14.4923
8 UUUUUUUUUUUU[8]	11	100	19.6	19.6448	14.5291	15.3131
9 GAAGAGAAGC[5]	1	110	48.85	47.8156	45.2586	47.1382
10 UUCUUUCUUUUC[6]	3	110	46.5	42.0605	37.2669	40.6122
11 CGCAAGAGAAACGC[2]	10	110	59.64	67.9921	64.0121	68.644
12 ACGCCACGUGA[4]	100	120	69	72.4696	65.6083	73.131
13 ACGCGACGUGA[4]	100	120	67.6	70.8136	64.0291	71.1855
14 ACGCUAUGUGA[4]	100	120	56.7	61.3654	54.3281	63.0262
15 ACGCUACGUGA[4]	100	120	62.5	67.488	60.2977	67.9226
16 ACGCAACGUGA[4]	100	120	61.2	65.9993	59.4782	66.8666
17 CUGGUCGCAUC[4]	100	120	66.8	67.5281	63.1521	69.1093
18 ACGCUAAGUGA[4]	100	120	56.4	62.5719	55.8479	63.2488
19 ACGCUAGGUGA[4]	100	120	64.5	69.2739	62.0365	69.7995
20 AAGUGAUC[3]	8	132	32.9	32.5768	31.4333	32.68
21 CGCUGUAA[3]	8	132	36.3	40.089	34.4359	39.4742
22 CACGGCUC[3]	8	132	45.5	54.544	51.7121	54.6333
23 GCCAGUUAA[3]	8	132	40.2	46.5151	40.6132	45.8724
24 CGCUGUUAC[3]	8	132	37.9	49.3485	46.7081	48.9873
25 AUUGGAUACAAA[3]	8	132	43.7	45.7366	39.7702	47.2476
$\langle \Delta T \rangle$				3.96 °C	3.62 °C	4.60 °C
χ^2				721.35 °C^2	473.23 °C^2	728.44 °C^2

Table S7. Interpolation coefficients for IP-FIF.

	enthalpy			entropy		
	c_1	c_2	c_3	c_1	c_2	c_3
AUpAU	28.039	-31.294	6.695	92.382	-100.905	21.716
AUpCG	-24.591	11.907	-2.663	-80.346	44.462	-9.674
AUpGC	-2.961	-6.552	1.387	-9.319	-17.202	3.879
AUpUA	-43.672	32.545	-7.346	-137.503	101.995	-22.631
CGpAU	39.380	-44.071	9.255	131.355	-141.445	29.855
CGpCG	-20.849	6.737	-1.436	-61.090	24.458	-5.038
CGpGC	11.312	-18.660	3.742	39.867	-57.619	11.691
GCpAU	-2.424	-9.575	1.976	-4.712	-27.910	5.887
GCpCG	-17.498	2.303	-0.455	-54.389	14.048	-2.680
UApAU	-39.518	25.541	-5.537	-123.922	82.510	-17.800

Table S8. Interpolation coefficients for IP-VIF.

	enthalpy			entropy		
	c_1	c_2	c_3	c_1	c_2	c_3
AUpAU	16.160	-20.241	4.303	61.729	-72.196	15.472
AUpCG	-22.373	9.163	-2.044	-68.487	32.262	-7.042
AUpGC	0.148	-10.050	2.063	4.829	-31.334	6.606
AUpUA	-5.774	-3.149	0.327	-33.277	5.175	-1.934
CGpAU	17.977	-24.100	4.912	91.839	-105.058	21.907
CGpCG	-52.998	35.622	-7.578	-140.879	95.829	-20.197
CGpGC	-1.918	-6.779	1.130	14.598	-35.236	6.682
GCpAU	-21.947	8.471	-1.820	-39.183	3.233	-0.520
GCpCG	-39.862	22.410	-4.709	-104.617	58.903	-12.139
UApAU	-32.065	18.690	-3.864	-69.342	30.374	-5.844
initiation	40.075	-32.421	6.865	29.639	-25.337	5.230
terminal AU	-28.390	30.011	-6.588	-79.605	83.525	-18.318

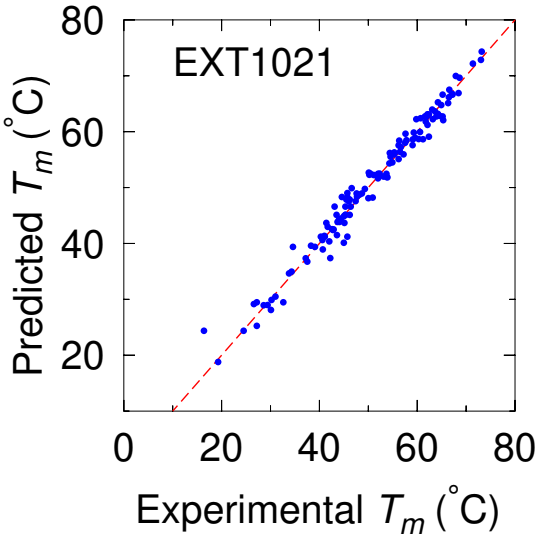

Figure S1. Scatterplots of the experimental versus predicted melting temperatures using the P-XIA98 parameters for the extended dataset D-RW-EXT1021.

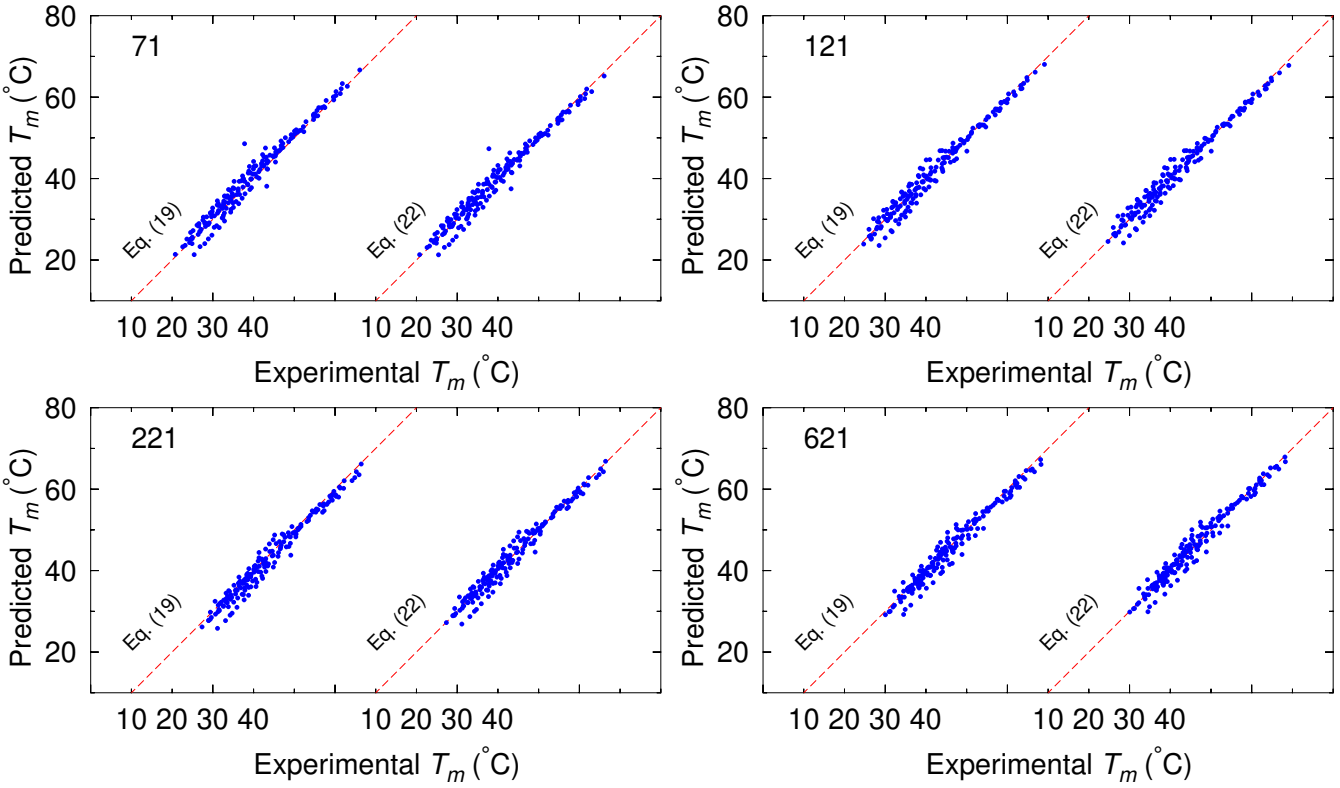

Figure S2. Scatterplots of the experimental versus predicted melting temperatures using the P-XIA98 parameters and salt corrections from Chen and Znosko [10]. Equation numbers refer to the salt correction used in reference 10.

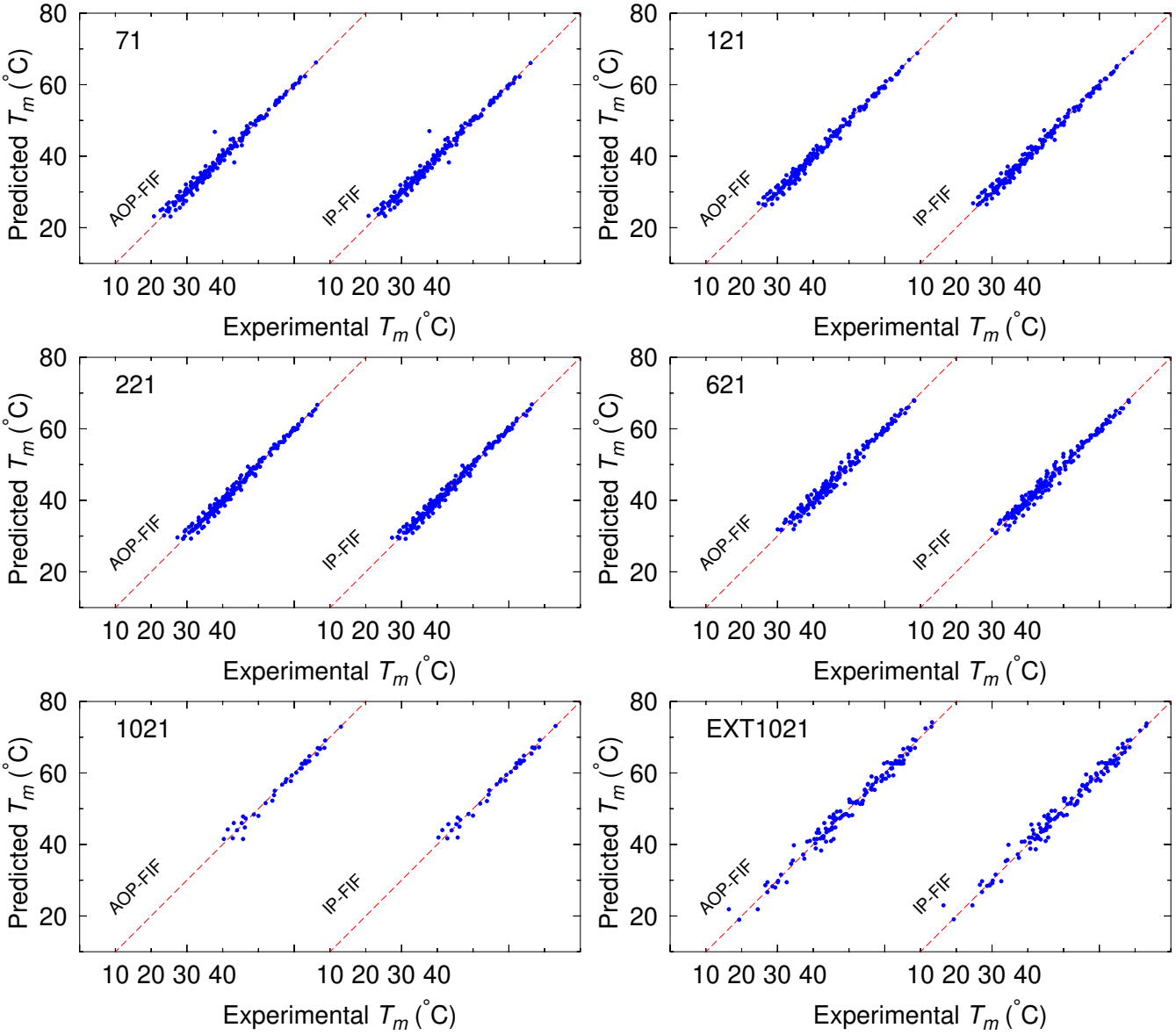

Figure S3. Scatterplots of the experimental versus predicted melting temperatures for the FIF scheme.

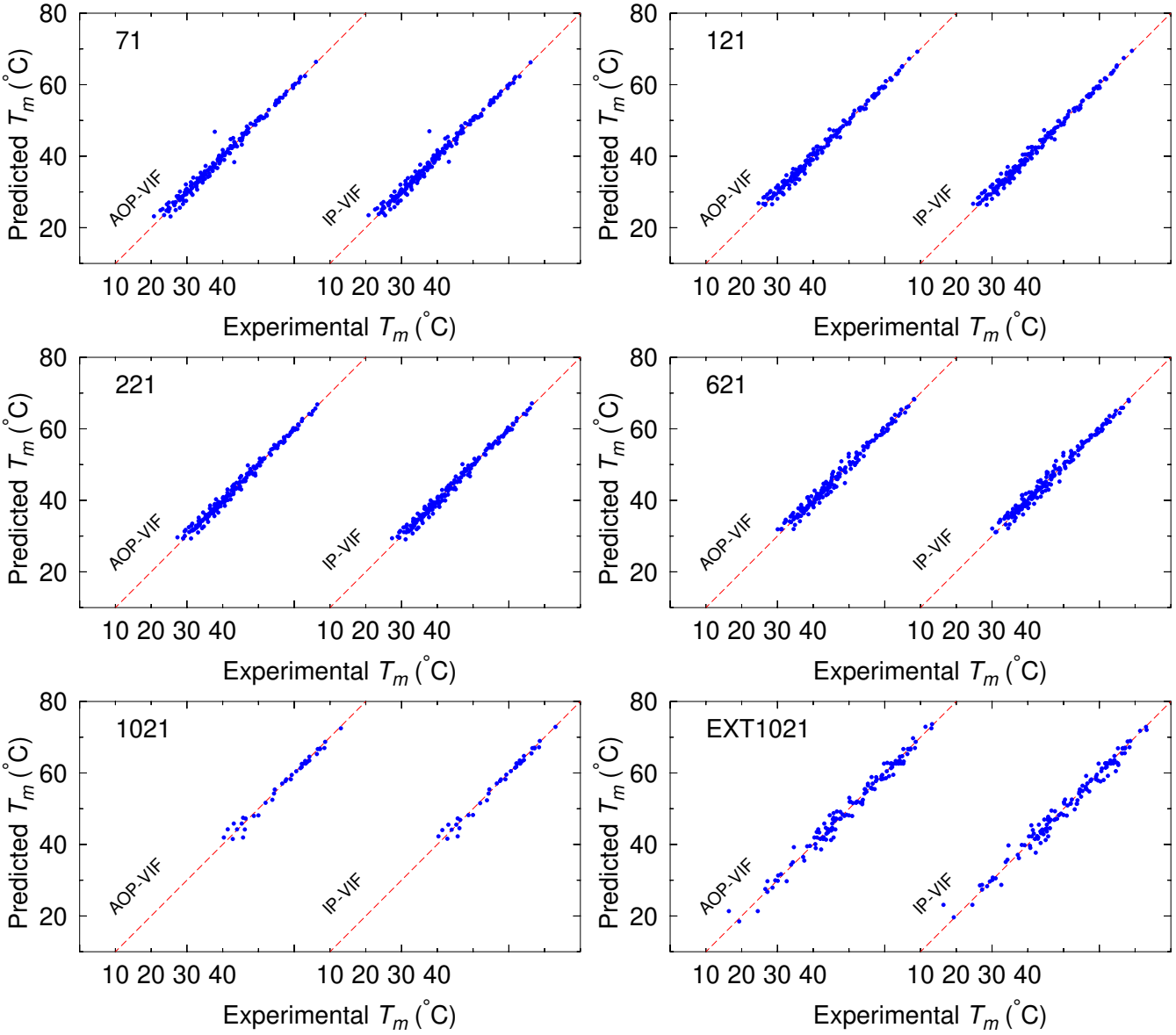

Figure S4. Scatterplots of the experimental versus predicted melting temperatures for the VIF scheme.

[1]G. T. Walker, "Deoxycytidine methylation does not affect DNA-RNA hybrid formation or B–A transitions of $(dG)_n.(dC)_n$ sequences," Nucleic Acids Res. **16**, 3091–3099 (1988).
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