

**Supp Table 3: Calculated binding affinities (nM) in MPSL for DQ 1-8**

Column1	Pos1	Pos2	Pos3	Pos4	Pos5	Pos6	Pos7	Pos8	Pos9
A	2894.9	2089.459	1438.348	1944.429	1511.42	1576.335	1756.85	1704.296	1376.391
C	2830.327	2620.236	2719.792	3201.379	2199.5	4091.521	2868.673	2824.166	2815.889
D	3084.427	2927.642	2760.198	2086.846	2491.68	2482.046	2150.758	2780.638	2417.291
E	2985.931	2941.337	3062.038	3007.646	3000.788	3826.526	3022.603	2496.679	2675.045
F	1903.794	1819.639	2227.472	2190.43	2301.782	2973.264	2281.599	2952.315	2693.699
G	3271.216	1851.125	1840.86	1754.407	1995.185	2010.827	1842.004	2319.221	2318.959
H	2467.511	1947.271	2287.26	2832.752	2453.913	3231.556	2611.153	2339.05	2152.601
I	1933.184	1535.998	1681.017	1654.476	1414.216	1707.18	1640.899	1694.551	1931.265
K	2613.402	2506.336	2284.314	3027.892	2203.438	3214.236	2158.448	2248.871	1558.9
L	1840.077	1581.427	2054.702	1577.016	1819.111	1798.527	1533.999	1854.671	1698.027
M	2286.36	1488.785	2030.05	1915.434	2042.83	1978.558	1564.975	1827.103	1750.202
N	2862.646	2333.008	2364.522	2212.115	2418.763	2069.194	2188.539	1885.696	2118.784
P	3904.442	2329.673	3325.118	2200.607	1830.258	1929.618	1994.464	2114.652	2430.06
Q	3224.107	2503.876	2914.499	2160.584	2310.519	2050.964	2133.464	1865.28	2175.147
R	3140.529	1986.39	2463.673	2907.617	2314.791	2427.874	2314.148	1951.356	2413.675
S	2936.655	1578.863	1528.49	1502.337	1481.485	1371.125	1438.338	1754.845	1813.967
T	2202.28	1961.924	2424.753	1806.134	1560.127	1625.071	1788.829	2139.174	2007.643
V	1640.296	1675.998	1244.793	1209.075	1282.902	1610.065	1651.289	1408.63	1675.399
W	1392.953	1570.844	1803.159	2132.914	2190.836	2151.511	2147.45	1594.775	1543.302
Y	1338.433	1607.486	1503.501	1874.59	2087.485	2537.318	2184.018	1739.449	1821.526