

Supp Table 7: Calculated binding affinities (nM) in MPSL for DQ *Neophocaena phocaenoides*

Column1	Pos1	Pos2	Pos3	Pos4	Pos5	Pos6	Pos7	Pos8	Pos9
A	927.8525	766.9142	537.4887	706.5051	439.0394	512.9451	518.8536	500.584	530.3664
C	940.6855	951.8627	990.3961	1254.929	777.1276	1513.093	1117.87	1005.015	1370.74
D	1065.673	935.7596	1323.689	699.1512	701.4269	807.742	716.4248	1082.235	834.375
E	1208.23	1003.455	1493.03	934.8286	1111.521	1519.361	1004.641	962.0808	1062.079
F	712.1897	653.6381	501.2475	708.0078	839.9533	894.3151	592.3894	803.1408	750.8771
G	1360.011	665.8372	560.5838	592.7609	624.5711	591.2742	806.5915	915.8832	928.1497
H	752.8596	597.9275	679.4167	775.8114	610.3952	1025.89	683.1279	658.8327	533.423
I	429.5332	335.4991	398.1927	449.3989	482.6957	520.5463	545.0217	527.3007	506.2175
K	910.7201	623.8836	612.1952	908.6821	674.5774	755.7168	629.0861	568.7866	430.0323
L	414.3455	408.5696	460.8306	411.3818	487.1678	494.8776	429.435	476.4447	439.3355
M	590.8654	571.6216	521.5206	478.6931	688.7746	512.3982	444.5653	502.909	392.0446
N	1096.729	681.4034	649.4024	639.4642	575.2374	517.7186	776.6732	651.7082	766.0999
P	1232.002	1091.099	1094.269	919.9004	611.5737	561.0192	693.5502	745.7815	864.3657
Q	1176.197	786.2841	777.7018	613.547	615.9477	624.3476	556.2376	566.4928	785.0512
R	1337.663	592.6207	695.6935	870.7756	698.7882	726.0022	660.3675	457.6693	683.2775
S	1011.681	533.1418	487.3978	480.9681	463.4491	449.0572	513.4564	655.4754	692.6561
T	800.7179	631.9815	700.0649	644.6907	664.654	407.2992	623.1111	693.9184	702.5435
V	466.8926	381.9504	388.7896	407.6047	424.16	538.4922	597.0757	471.7449	550.9233
W	572.9013	673.9976	607.6605	585.0058	660.0692	725.4737	650.5403	489.4848	429.482
Y	496.1744	533.262	490.6804	564.006	582.0191	837.4741	621.262	657.6894	582.9244