

## Supporting Information for Andrews and Bray, Stochastic Simulation of Chemical Reactions with Spatial Resolution and Single Molecule Detail.

Table S1. Reaction rates for irreversible reactions using the bimolecular reaction algorithm presented in the paper. The experimental bimolecular reaction rate,  $k$ , is made unitless by reducing it to  $k\Delta t/\bar{\square}_b^3$ , where  $\Delta t$  is the simulation time step and  $\bar{\square}_b$  is the simulation binding radius. Mutual rms step lengths,  $s$ , are reduced to  $s'=s/\bar{\square}_b$ . The reduced reaction rates shown here are averages (means) of those that were calculated with  $s'$  values that were sequentially decreased from 20.0855 ( $e^3$ ) to 0.0498 ( $e^{-3}$ ) and those that were increased over the same range. The deviations column reports the differences between these two sets of raw data; errors in the averaged data are expected to be less than half of the deviations.

$s'$	$k\Delta t/\bar{\square}_b^3$	deviations
20.0855	4.1886	0.0000
16.4446	4.1884	0.0000
13.4637	4.1880	0.0000
11.0232	4.1871	0.0000
9.0250	4.1855	0.0000
7.3891	4.1822	0.0000
6.0496	4.1762	0.0000
4.9530	4.1653	0.0000
4.0552	4.1462	0.0003
3.3201	4.1127	0.0007
2.7183	4.0542	0.0010
2.2255	3.9541	0.0014
1.8221	3.7900	0.0019
1.4918	3.5368	0.0026
1.2214	3.1783	0.0033
1.0000	2.7240	0.0041
0.8187	2.2178	0.0048
0.6703	1.7221	0.0054
0.5488	1.2875	0.0058
0.4493	0.9366	0.0062
0.3679	0.6682	0.0065
0.3012	0.4700	0.0066
0.2466	0.3271	0.0064
0.2019	0.2259	0.0057
0.1653	0.1551	0.0046
0.1353	0.1061	0.0035
0.1108	0.0724	0.0026
0.0907	0.0492	0.0019
0.0743	0.0334	0.0014
0.0608	0.0226	0.0010
0.0498	0.0153	0.0007

Table S2. Reduced reaction rates for reversible reactions for various values of the reduced rms step length ( $s$ ) and the reduced unbinding radius ( $\bar{\Omega}_i = \bar{\Omega}_i / \bar{\Omega}_0$ ) with  $\bar{\Omega}_i \geq 1$ , calculated as for table S1. Differences between results calculated with increasing and decreasing  $s$  values were always less than 0.001 except for those numbers marked with an asterisk. In all cases, differences were less than 0.01.

$s$	20.0855	16.4446	13.4637	11.0232	9.0250	7.3891	6.0496	4.9530	4.0552	3.3201	2.7183	2.2255	1.8221	1.4918	1.2214	1.0000
20.0855	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1887	4.1887	4.1887
16.4446	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1887	4.1887	4.1887	4.1886	4.1885
13.4637	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1887	4.1887	4.1887	4.1886	4.1886	4.1884	4.1883	4.1882
11.0232	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1887	4.1887	4.1886	4.1885	4.1884	4.1884	4.1880	4.1877	4.1875
9.0250	4.1888	4.1888	4.1888	4.1888	4.1887	4.1887	4.1886	4.1886	4.1884	4.1882	4.1880	4.1877	4.1873	4.1869	4.1865	4.1862
7.3891	4.1888	4.1888	4.1887	4.1887	4.1886	4.1885	4.1884	4.1881	4.1878	4.1873	4.1868	4.1861	4.1854	4.1848	4.1842	4.1837
6.0496	4.1887	4.1887	4.1886	4.1885	4.1883	4.1880	4.1876	4.1870	4.1862	4.1852	4.1840	4.1828	4.1817	4.1806	4.1797	4.1789
4.9530	4.1887	4.1885	4.1883	4.1879	4.1874	4.1867	4.1856	4.1842	4.1825	4.1805	4.1783	4.1762	4.1743	4.1726	4.1712	4.1700
4.0552	4.1884	4.1880	4.1874	4.1864	4.1851	4.1833	4.1809	4.1779	4.1745	4.1707	4.1669	4.1633	4.1601	4.1574	4.1553*	4.1535*
3.3201	4.1878	4.1867	4.1851	4.1828	4.1796	4.1756	4.1705	4.1645	4.1579	4.1509	4.1442	4.1383	4.1334*	4.1296*	4.1264*	4.1237*
2.7183	4.1864	4.1835	4.1796	4.1744	4.1675	4.1589	4.1485	4.1366	4.1239	4.1116	4.1008	4.0921*	4.0850*	4.0792*	4.0745*	4.0705*
2.2255	4.1830	4.1764	4.1677	4.1561	4.1414	4.1232	4.1020	4.0792	4.0569	4.0376*	4.0218*	4.0092*	3.9989*	3.9905*	3.9836*	3.9779*
1.8221	4.1755	4.1609	4.1415	4.1162	4.0846	4.0473	4.0069	3.9679*	3.9340*	3.9067*	3.8849*	3.8672*	3.8528*	3.8410*	3.8314*	3.8234*
1.4918	4.1587	4.1259	4.0827	4.0284	3.9646	3.8960	3.8299*	3.7729*	3.7273*	3.6912*	3.6622*	3.6387*	3.6197*	3.6043*	3.5916*	3.5810*
1.2214	4.1196	4.0473	3.9568	3.8515	3.7395*	3.6325*	3.5412*	3.4687*	3.4121*	3.3673*	3.3314*	3.3026*	3.2793*	3.2605*	3.2451*	3.2320*
1.0000	4.0367	3.8900	3.7224*	3.5469*	3.3818*	3.2422*	3.1333*	3.0501*	2.9854*	2.9344*	2.8939*	2.8617*	2.8358*	2.8149*	2.7977*	2.7833*
0.8187	3.8834	3.6218	3.3557*	3.1102*	2.9064*	2.7510*	2.6357*	2.5487*	2.4816*	2.4293*	2.3881*	2.3554*	2.3293*	2.3082*	2.2909*	2.2770*
0.6703	3.6411	3.2374	2.8780*	2.5879*	2.3730*	2.2202*	2.1096*	2.0269*	1.9639*	1.9152*	1.8771*	1.8470*	1.8229*	1.8037*	1.7883*	1.7760*
0.5488	3.3169	2.7736	2.3537*	2.0556*	1.8544*	1.7172*	1.6193*	1.5470*	1.4925*	1.4507*	1.4181*	1.3924*	1.3720*	1.3560*	1.3432*	1.3331*
0.4493	2.9457	2.2892	1.8508*	1.5749*	1.4013*	1.2857*	1.2043*	1.1450*	1.1005*	1.0666*	1.0404*	1.0198*	1.0037*	0.9910*	0.9810*	0.9731*
0.3679	2.5661	1.8317	1.4114*	1.1746*	1.0326*	0.9397*	0.8752*	0.8286*	0.7940*	0.7677*	0.7475*	0.7318*	0.7196*	0.7099*	0.7023*	0.6963*
0.3012	2.2039	1.4275	1.0509*	0.8583*	0.7465*	0.6745*	0.6252*	0.5899*	0.5638*	0.5441*	0.5291*	0.5174*	0.5083*	0.5012*	0.4955*	0.4911*
0.2466	1.8729	1.0874	0.7680*	0.6172*	0.5318*	0.4776*	0.4409*	0.4148*	0.3956*	0.3812*	0.3702*	0.3617*	0.3551*	0.3499*	0.3459*	0.3427*
0.2019	1.5787	0.8119	0.5531*	0.4382*	0.3744*	0.3346*	0.3078*	0.2889*	0.2751*	0.2647*	0.2568*	0.2508*	0.2460*	0.2423*	0.2394*	0.2372*
0.1653	1.3225	0.5957	0.3935*	0.3078*	0.2612*	0.2325*	0.2132*	0.1997*	0.1899*	0.1826*	0.1770*	0.1727*	0.1693*	0.1667*	0.1647*	0.1631*
0.1353	1.1030	0.4310	0.2771*	0.2144*	0.1809*	0.1604*	0.1468*	0.1373*	0.1304*	0.1252*	0.1213*	0.1183*	0.1160*	0.1142*	0.1128*	0.1117*
0.1108	0.9168	0.3080	0.1935*	0.1484	0.1246	0.1101	0.1006	0.0939*	0.0891*	0.0855*	0.0828*	0.0807*	0.0791*	0.0779*	0.0769*	0.0762*
0.0907	0.7600*	0.2180	0.1342	0.1021	0.0853	0.0752	0.0686	0.0640	0.0607	0.0582*	0.0563*	0.0549*	0.0538*	0.0529*	0.0523*	0.0518*
0.0743	0.6285*	0.1530	0.0925	0.0699	0.0582	0.0512	0.0467	0.0435	0.0412	0.0395	0.0382	0.0372	0.0365*	0.0359*	0.0355*	0.0352*
0.0608	0.5190*	0.1066	0.0635	0.0477	0.0396	0.0348	0.0316	0.0295	0.0279	0.0267	0.0259	0.0252	0.0247	0.0243	0.0240	0.0238
0.0498	0.4281*	0.0738	0.0434	0.0324	0.0269	0.0236	0.0214	0.0199	0.0189	0.0181	0.0175	0.0170	0.0167	0.0164	0.0162	0.0161

Table S3. Reduced reaction rates for reversible reactions for various values of the reduced rms step length ( $s'$ ) and the reduced unbinding radius ( $\bar{r}_u'$ ) with  $\bar{r}_u' \leq 1$ , calculated as for table S1. Calculations could only be carried out with decreasing  $s'$  values, so errors are not estimated here. A hyphen indicates that the reduced reaction rate was still changing by more than  $10^{-5}$  after each iteration, after a total of  $10^5$  iterations on the respective  $s'$  value.

$s'$	$\bar{r}_u'$										
	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
20.0855	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
16.4446	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
13.4637	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
11.0232	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
9.0250	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
7.3891	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888
6.0496	4.1889	4.1889	4.1889	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1888	4.1887
4.9530	4.1890	4.1890	4.1890	4.1890	4.1889	4.1889	4.1889	4.1888	4.1888	4.1887	4.1887
4.0552	4.1893	4.1893	4.1892	4.1892	4.1891	4.1890	4.1890	4.1889	4.1888	4.1886	4.1884
3.3201	4.1902	4.1901	4.1900	4.1900	4.1898	4.1896	4.1893	4.1890	4.1887	4.1883	4.1879
2.7183	4.1922	4.1922	4.1917	4.1913	4.1908	4.1902	4.1894	4.1894	4.1886	4.1877	4.1866
2.2255	4.1969	4.1967	4.1963	4.1957	4.1947	4.1935	4.1921	4.1903	4.1884	4.1862	4.1838
1.8221	4.2082	4.2079	4.2069	4.2052	4.2030	4.2000	4.1965	4.1924	4.1878	4.1826	4.1770
1.4918	4.2370	4.2361	4.2336	4.2294	4.2236	4.2163	4.2075	4.1973	4.1860	4.1735	4.1601
1.2214	4.3077	4.3055	4.2990	4.2882	4.2735	4.2550	4.2331	4.2083	4.1809	4.1515	4.1205
1.0000	4.4735	4.4679	4.4512	4.4241	4.3873	4.3421	4.2898	4.2318	4.1696	4.1046	4.0381
0.8187	4.8528	4.8381	4.7951	4.7263	4.6353	4.5269	4.4061	4.2775	4.1458	4.0143	3.8862
0.6703	5.7236	5.6831	5.5660	5.3845	5.1557	4.8979	4.6280	4.3596	4.1027	3.8633	3.6451
0.5488	7.8386	7.7105	7.3528	6.8319	6.2281	5.6102	5.0255	4.4993	4.0411	3.6506	3.3221
0.4493	13.8800	13.3567	11.9944	10.2420	8.4948	6.9661	5.7193	4.7387	3.9808	3.3987	2.9519
0.3679	40.3625	36.4825	28.0859	19.9323	13.840	9.7043	6.9732	5.1687	3.9619	3.1412	2.5731
0.3012	-	-	261.8342	69.5815	30.7080	16.1829	9.4547	5.9735	4.0396	2.9062	2.2121
0.2466	-	-	-	-	217.6851	37.7789	15.1652	7.5541	4.2921	2.7137	1.8833
0.2019	-	-	-	-	-	387.1930	32.6698	10.9749	4.8587	2.5802	1.5922
0.1653	-	-	-	-	-	-	175.5054	20.0157	6.0450	2.5241	1.3398
0.1353	-	-	-	-	-	-	-	59.7297	8.6721	2.5741	1.1242
0.1108	-	-	-	-	-	-	-	-	15.7043	2.7854	0.9426
0.0907	-	-	-	-	-	-	-	-	48.4378	3.2783	0.7914
0.0743	-	-	-	-	-	-	-	-	-	4.3506	0.6671
0.0608	-	-	-	-	-	-	-	-	-	6.8976	0.5668
0.0498	-	-	-	-	-	-	-	-	-	14.9241	0.4879