Supplementary Information

Binding Data

Table S1. Binding data for the MAA-polymer series.

Polymer	Molar ratio [a]	B/T_MIP	B/T_REF	B/T_Spec
0	1:0:56	−0.0365	0.0029	−0.0395
		−0.0163	0.0224	−0.0387
		0.0007	0.0387	−0.0381
		−0.0029	−0.0763	0.0734
		0.0167	−0.0552	0.0719
		0.0331	−0.0376	0.0707
		−0.0099	−0.0090	−0.0010
		0.0098	0.0107	−0.0009
		0.0263	0.0272	−0.0009
1	1:2:56	0.1342	−0.0178	0.1520
		0.1716	0.0261	0.1454
		0.1662	0.0198	0.1464
		0.1486	−0.0155	0.1642
		0.1854	0.0283	0.1571
		0.1801	0.0220	0.1581
		0.1818	−0.0154	0.1972
		0.2171	0.0285	0.1886
		0.2120	0.0221	0.1899
2	1:5:54	0.2509	0.0132	0.2377
		0.2379	−0.0040	0.2419
		0.2550	0.0185	0.2365
		0.2562	0.0180	0.2382
		0.2433	0.0009	0.2424
		0.2603	0.0233	0.2369
		0.2639	0.0080	0.2559
		0.2511	−0.0093	0.2603
		0.2679	0.0134	0.2545
3	1:9:56	0.4505	0.0459	0.4046
		0.4623	0.0664	0.3959
		0.4570	0.0571	0.3998
		0.4330	0.0479	0.3851
		0.4452	0.0684	0.3768
		0.4397	0.0591	0.3806
		0.4516	0.0592	0.3924
		0.4634	0.0794	0.3840
		0.4581	0.0703	0.3878

Table S1. *Cont.*

Polymer	Molar ratio [a]	B/T_MIP	B/T_REF	B/T_Spec
		0.2765	0.0639	0.2126
		0.2846	0.0744	0.2102
		0.2796	0.0679	0.2117
		0.3228	0.0550	0.2678
4	1:12:56	0.3304	0.0657	0.2647
		0.3257	0.0591	0.2666
		0.3365	0.0565	0.2799
		0.3439	0.0672	0.2768
		0.3393	0.0606	0.2787
		0.5103	0.0790	0.4313
		0.5115	0.0812	0.4302
		0.5121	0.0825	0.4296
		0.5096	0.0725	0.4371
5	1:14:59	0.5108	0.0748	0.4360
		0.5114	0.0760	0.4354
		0.5205	0.0691	0.4513
		0.5216	0.0714	0.4502
		0.5223	0.0727	0.4496
		0.4191	0.0381	0.3810
		0.4221	0.0429	0.3791
		0.4200	0.0395	0.3805
		0.4531	0.0595	0.3936
6	1:16:56	0.4558	0.0642	0.3916
		0.4538	0.0608	0.3930
		0.4360	0.0749	0.3611
		0.4389	0.0795	0.3593
		0.4368	0.0762	0.3606
		0.3806	0.0781	0.3025
		0.3820	0.0801	0.3018
		0.3774	0.0733	0.3041
		0.4115	0.1136	0.2979
7	1:18:56	0.4128	0.1156	0.2973
		0.4085	0.1090	0.2995
		0.3758	0.1034	0.2724
		0.3772	0.1054	0.2718
		0.3726	0.0988	0.2738
		0.5078	0.1205	0.3873
		0.4952	0.0979	0.3973
		0.5241	0.1496	0.3745
		0.5004	0.1230	0.3774
8	1:22:59	0.4875	0.1005	0.3871
		0.5169	0.1520	0.3649
		0.5454	0.0948	0.4506
		0.5337	0.0716	0.4622
		0.5604	0.1248	0.4357

Table S1. *Cont.*

Polymer	Molar ratio [a]	B/T_MIP	B/T_REF	B/T_Spec
		0.5345	0.1643	0.3702
		0.5343	0.1640	0.3704
		0.5320	0.1597	0.3723
		0.5094	0.1733	0.3360
9	1:46:55	0.5092	0.1730	0.3362
		0.5067	0.1688	0.3379
		0.5425	0.1480	0.3945
		0.5424	0.1477	0.3947
		0.5400	0.1434	0.3967

[a] Bupivacaine:MAA:EGDMA.

Table S2. Binding data for the MMA-polymer series.

Polymer	Molar ratio [a]	B/T_MIP	B/T_REF	B/T_Spec
		−0.0283	0.0014	−0.0297
		−0.0239	0.0057	−0.0296
		−0.0202	0.0092	−0.0295
		−0.0386	−0.0034	−0.0352
10	1:7:56	−0.0342	0.0008	−0.0350
		−0.0305	0.0044	−0.0349
		−0.0543	0.0034	−0.0577
		−0.0498	0.0076	−0.0574
		−0.0461	0.0112	−0.0572
		0.0017	−0.0067	0.0084
		0.0152	0.0070	0.0082
		0.0035	−0.0048	0.0083
		−0.0060	−0.0134	0.0073
11	1:9:56	0.0076	0.0004	0.0072
		−0.0042	−0.0115	0.0073
		−0.0087	−0.0174	0.0087
		0.0050	−0.0036	0.0086
		−0.0068	−0.0155	0.0087
		0.0062	0.0020	0.0042
		0.0127	0.0086	0.0041
		0.0139	0.0098	0.0041
		0.0196	−0.0058	0.0254
12	1:12:56	0.0261	0.0009	0.0252
		0.0272	0.0021	0.0252
		0.0009	0.0046	−0.0037
		0.0075	0.0112	−0.0037
		0.0087	0.0124	−0.0037

Table S2. *Cont.*

Polymer	Molar ratio [a]	B/T_MIP	B/T_REF	B/T_Spec
13	1:14:56	0.0161	0.0046	0.0115
		0.0051	−0.0065	0.0116
		0.0200	0.0085	0.0115
		0.0130	−0.0045	0.0175
		0.0020	−0.0157	0.0177
		0.0169	−0.0006	0.0174
		0.0167	−0.0052	0.0219
		0.0057	−0.0165	0.0222
		0.0205	−0.0013	0.0218
14	1:22:56	0.0144	0.0186	−0.0042
		0.0104	0.0147	−0.0042
		0.0117	0.0159	−0.0042
		0.0239	0.0210	0.0029
		0.0199	0.0170	0.0029
		0.0212	0.0183	0.0029
		0.0288	0.0029	0.0259
		0.0249	−0.0012	0.0260
		0.0261	0.0001	0.0260
15	1:46:56	−0.0025	−0.0149	0.0123
		0.0124	0.0003	0.0121
		0.0009	−0.0114	0.0123
		−0.0056	−0.0072	0.0017
		0.0094	0.0078	0.0017
		−0.0021	−0.0038	0.0017
		0.0018	0.0099	−0.0081
		0.0167	0.0247	−0.0080
		0.0053	0.0134	−0.0081

[a] Bupivacaine:MMA:EGDMA.

Morphology Analysis

Table S3. Surface areas of the studied MAA-polymer series derived with the BET- and Langmuir methods together with the corresponding pore volumes.

Polymer	BET-Surface Area (m^2/g) [*r*] [a]	Langmuir Surface Area (m^2/g) [*r*] [a]	Pore Volume [b] (cm^3/g)
MIP 0	542.8 ± 4.0 [1.000]	748.1 ± 21.3 [0.998]	1.206078
REF 0	464.9 ± 6.5 [1.000]	703.1 ± 28.7 [0.997]	1.589258
MIP 1	339.0 ± 3.6 [1.000]	470.1 ± 9.3 [0.999]	0.838057
REF 1	319.0 ± 1.5 [1.000]	439.7 ± 11.3 [0.999]	0.750579
MIP 2	380.7 ± 1.9 [1.000]	528.1 ± 14.0 [0.999]	0.955491
REF 2	358.4 ± 1.6 [1.000]	493.9 ± 13.0 [0.999]	0.900607
MIP 3	381.6 ± 3.1 [1.000]	529.2 ± 12.5 [0.999]	0.959272
REF 3	275.2 ± 1.8 [1.000]	378.9 ± 4.0 [0.999]	0.671729
MIP 4	357.5 ± 2.4 [1.000]	491.5 ± 11.8 [1.000]	0.905193
REF 4	233.6 ± 2.1 [1.000]	323.8 ± 6.5 [0.999]	0.564389
MIP 5	315.1 ± 1.9 [1.000]	437.1 ± 10.5 [0.999]	0.908728
REF 5	324.0 ± 1.7 [1.000]	449.1 ± 12.3 [0.999]	0.870039

Table S3. *Cont.*

Polymer	BET-Surface Area (m^2/g) [*r*] [a]	Langmuir Surface Area (m^2/g) [*r*] [a]	Pore Volume [b] (cm^3/g)
MIP 6	306.8 ± 4.2 [1.000]	426.4 ± 7.1 [0.999]	0.751675
REF 6	121.1 ± 0.5 [1.000]	168.7 ± 4.6 [0.998]	0.319340
MIP 7	179.6 ± 0.5 [1.000]	250.5 ± 7.1 [0.998]	0.580967
REF 7	220.7 ± 1.0 [1.000]	306.5 ± 8.6 [0.998]	0.622254
MIP 8	284.8 ± 1.1 [1.000]	395.2 ± 10.3 [0.999]	0.762485
REF 8	272.6 ± 2.2 [1.000]	376.6 ± 9.3 [0.999]	0.736557
MIP 9	79.6 ± 0.3 [1.000]	110.3 ± 3.6 [0.998]	0.290185
REF 9	75.0 ± 0.6 [1.000]	105.2 ± 2.7 [0.999]	0.225999

[a] Areas presented as mean ± standard deviation from linear regression where *r* is the correlation coefficient.

[b] Single point total pore volume.

Table S4. Surface areas of the studied MMA-polymer series derived with the BET- and Langmuir methods together with the corresponding pore volumes.

Polymer	BET-Surface Area (m^2/g) [*r*] [a]	Langmuir Surface Area (m^2/g) [*r*] [a]	Pore Volume [b] (cm^3/g)
MIP 10	493.3 ± 2.9 [9.999]	679.5 ± 18.2 [9.986]	1.153493
REF 10	458.3 ± 2.5 [9.999]	631.7 ± 16.3 [9.987]	1.083441
MIP 11	476.5 ± 2.5 [9.999]	656.7 ± 17.8 [9.999]	1.138099
REF 11	429.0 ± 1.7 [1.000]	591.9 ± 17.2 [9.985]	1.304587
MIP 12	482.9 ± 2.9 [9.999]	666.9 ± 17.6 [9.986]	1.157097
REF 12	397.5 ± 2.3 [9.999]	550.7 ± 15.0 [9.985]	1.192906
MIP 13	465.6 ± 2.7 [9.999]	642.5 ± 17.2 [9.986]	1.111784
REF 13	378.8 ± 1.9 [9.999]	524.6 ± 13.5 [9.987]	1.145409
MIP 14	432.1 ± 2.3 [9.999]	597.4 ± 16.2 [9.985]	1.102891
REF 14	387.7 ± 2.6 [9.999]	538.1 ± 16.2 [9.982]	0.975367
MIP 15	328.8 ± 1.0 [1.000]	456.3 ± 12.6 [9.985]	0.995139
REF 15	317.2 ± 0.9 [1.000]	440.3 ± 13.1 [9.982]	1.008397

[a] Areas presented as mean ± standard deviation from linear regression where r is the correlation coefficient.

[b] Single point total pore volume.

Swelling Study

Table S5. Swelling ratio (%) for the MAA-polymer series.

Polymer	0	1	2	3	4	5	6	7	8	9
MIP	40	80	80	50	50	70	30	60	30	60
REF	80	80	80	40	40	40	40	40	80	60

Table S6. Swelling ratio (%) for the MMA-polymer series.

Polymer	10	11	12	13	14	15
MIP	30	40	40	60	60	70
REF	50	60	60	70	40	60

MD—Composition of the Simulated Pre-Polymerization Mixtures

Table S7. Composition of the simulated MAA-MIP pre-polymerization mixtures. Each system was simulated in quintuplicate totally covering 50 ns of recorded trajectory data for each pre-polymerization mixture.

System	Number of Molecules					Molar Ratio				
	Bupivacaine	MAA	EGDMA	AIBN	Toluene	Bupivacaine	MAA	EGDMA	AIBN [a]	Toluene [b]
S0	10	0	557	14	891	1	0.0	55.7	1.3	1.6
S1	10	24	557	15	930	1	2.4	55.7	1.3	1.6
S2	10	52	557	15	974	1	5.2	55.7	1.3	1.6
S3	10	90	557	16	1035	1	9.0	55.7	1.3	1.6
S4	10	120	557	16	1083	1	12.0	55.7	1.3	1.6
S5	10	144	557	16	1122	1	14.4	55.7	1.3	1.6
S6	10	160	557	17	1147	1	16.0	55.7	1.3	1.6
S7	10	180	557	17	1179	1	18.0	55.7	1.3	1.6
S8	10	222	557	17	1246	1	22.2	55.7	1.3	1.6
S9	10	462	557	20	1630	1	46.2	55.7	1.3	1.6

[a] Mol-% of the total amount of polymerizable methacrylate units present in the mixtures. [b] Times the total volume of the monomers.

Table S8. Composition of the simulated MMA-MIP pre-polymerization mixtures. Each system was simulated in quintuplicate totally covering 50 ns of recorded trajectory data for each pre-polymerization mixture.

System	Number of Molecules					Molar Ratio				
	Bupivacaine	MMA	EGDMA	AIBN	Toluene	Bupivacaine	MMA	EGDMA	AIBN [a]	Toluene [b]
S10	10	74	557	15	1010	1	7.4	55.7	1.3	1.6
S11	10	90	557	16	1035	1	9.0	55.7	1.3	1.6
S12	10	120	557	16	1083	1	12.0	55.7	1.3	1.6
S13	10	144	557	16	1122	1	14.4	55.7	1.3	1.6
S14	10	222	557	17	1246	1	22.2	55.7	1.3	1.6
S15	10	462	557	20	1630	1	46.2	55.7	1.3	1.6

[a] Mol-% of the total amount of polymerizable methacrylate units present in the mixtures. [b] Times the total volume of the monomers.

Equilibration and Production Run Data

Table S9. Thermodynamic properties for the different MAA-systems studied.

System	ρ (g/cm^3)	Temp. (K)	Volume (Å^3)	Energies (kcal/mol)		
				E_{POT}	E_{KIN}	E_{TOT}
S0_1	0.97	293.08 ± 1.55	69.59 × 69.59 × 69.59	10235.56 ± 123.67	21545.60 ± 113.96	31781.16 ± 171.28
S0_2	0.98	293.13 ± 1.50	69.54 × 69.54 × 69.54	10179.13 ± 115.59	21549.24 ± 110.13	31728.37 ± 155.56
S0_3	0.97	293.06 ± 1.52	69.65 × 69.65 × 69.66	10313.14 ± 118.64	21543.85 ± 111.97	31856.99 ± 163.22
S0_4	0.98	293.18 ± 1.52	69.55 × 69.55 × 69.55	10208.25 ± 117.44	21552.36 ± 111.82	31760.61 ± 161.53
S0_5	0.98	293.08 ± 1.50	69.55 × 69.55 × 69.55	10191.70 ± 121.77	21544.88 ± 110.18	31736.58 ± 162.82
S1_1	0.98	293.00 ± 1.47	70.22 × 70.22 × 70.22	9624.51 ± 118.77	22186.36 ± 111.61	31810.87 ± 159.11
S1_2	0.97	293.09 ± 1.52	70.34 × 70.34 × 70.34	9736.04 ± 122.41	22193.39 ± 115.12	31929.43 ± 169.49

Table S9. *Cont.*

System	ρ (g/cm^3)	Temp. (K)	Volume (Å^3)	Energies (kcal/mol)		
				E_{POT}	E_{KIN}	E_{TOT}
S1_3	0.97	293.18 ± 1.49	70.28 × 70.28 × 70.29	9699.57 ± 119.33	22199.87 ± 113.01	31899.43 ± 163.29
S1_4	0.97	293.14 ± 1.50	70.31 × 70.31 × 70.31	9728.02 ± 124.13	22197.03 ± 113.89	31925.05 ± 169.75
S1_5	0.97	293.11 ± 1.47	70.28 × 70.28 × 70.28	9666.92 ± 117.72	22194.81 ± 111.37	31861.72 ± 158.51
S2_1	0.97	293.09 ± 1.51	71.05 × 71.05 × 71.05	9042.94 ± 124.03	22912.30 ± 118.21	31955.24 ± 174.41
S2_2	0.97	293.08 ± 1.47	71.03 × 71.03 × 71.03	9009.96 ± 122.85	22911.39 ± 115.23	31921.34 ± 168.28
S2_3	0.97	293.04 ± 1.46	71.03 × 71.03 × 71.03	9036.38 ± 121.45	22908.26 ± 114.47	31944.64 ± 165.48
S2_4	0.97	293.10 ± 1.50	71.01 × 71.01 × 71.01	9035.55 ± 123.95	22912.67 ± 116.95	31948.22 ± 137.31
S2_5	0.97	293.06 ± 1.47	71.06 × 71.06 × 71.09	9057.17 ± 125.10	22910.03 ± 114.82	31967.20 ± 169.23
S3_1	0.97	293.10 ± 1.43	72.12 × 72.12 × 72.12	8229.79 ± 124.95	23919.87 ± 116.89	32149.66 ± 168.50
S3_2	0.97	293.09 ± 1.44	72.11 × 72.11 × 72.11	8212.24 ± 124.39	23918.65 ± 117.71	32130.89 ± 168.69
S3_3	0.97	293.05 ± 1.43	72.07 × 72.07 × 72.07	8144.35 ± 121.34	23915.62 ± 116.53	32059.97 ± 169.03
S3_4	0.97	293.06 ± 1.48	72.13 × 72.13 × 72.13	8210.11 ± 128.66	23916.21 ± 120.95	32126.32 ± 180.96
S3_5	0.97	293.13 ± 1.44	72.05 × 72.05 × 72.05	8131.65 ± 127.37	23921.87 ± 117.98	32053.52 ± 173.49
S4_1	0.96	293.05 ± 1.40	74.03 × 74.03 × 74.03	7901.32 ± 127.95	25772.13 ± 122.98	33673.45 ± 176.89
S4_2	0.97	293.08 ± 1.42	72.93 × 72.92 × 72.94	7555.27 ± 126.04	24697.27 ± 119.63	32252.54 ± 172.67
S4_3	0.97	293.00 ± 1.42	72.92 × 72.92x72 × 92	7520.54 ± 127.28	24690.17 ± 119.53	32210.71 ± 174.59
S4_4	0.97	293.03 ± 1.43	72.87 × 72.88 × 72.87	7489.02 ± 127.67	24693.20 ± 120.11	32182.21 ± 175.40
S4_5	0.97	293.01 ± 1.40	72.94 × 72.94 × 72.94	7578.07 ± 126.48	24691.44 ± 118.03	32269.51 ± 169.60
S5_1	0.97	293.07 ± 1.43	73.54 × 73.54 × 73.54	6988.73 ± 130.98	25325.84 ± 123.35	32314.56 ± 181.01
S5_2	0.96	293.02 ± 1.40	73.62 × 73.62 × 73.62	7057.53 ± 131.05	25322.07 ± 120.96	32379.60 ± 177.09
S5_3	0.97	293.13 ± 1.41	73.52 × 73.52 × 73.52	6983.36 ± 128.66	25331.83 ± 121.64	32315.19 ± 177.42
S5_4	0.97	293.06 ± 1.42	73.60 × 73.60 × 73.60	7035.97 ± 127.00	25325.71 ± 122.77	32361.68 ± 171.92
S5_5	0.97	293.06 ± 1.43	73.50 × 73.50 × 73.50	6941.49 ± 131.73	25325.17 ± 123.30	32266.66 ± 182.22
S6_1	0.97	293.03 ± 1.40	73.90 × 73.90 × 73.90	6581.01 ± 131.45	25749.24 ± 122.62	32330.26 ± 179.88
S6_2	0.97	293.02 ± 1.41	73.99 × 73.99 × 73.99	6639.57 ± 132.79	25748.44 ± 124.15	32388.01 ± 184.59
S6_3	0.97	293.03 ± 1.40	73.97 × 73.97 × 73.97	6638.83 ± 130.00	25749.28 ± 123.21	32388.11 ± 179.85
S6_4	0.97	293.04 ± 1.38	73.94 × 73.94 × 73.94	6615.20 ± 131.84	25750.48 ± 121.44	32365.68 ± 178.35
S6_5	0.97	293.00 ± 1.38	74.00 × 73.99 × 74.00	6665.94 ± 126.67	25746.99 ± 121.09	32412.93 ± 171.91
S7_1	0.97	292.96 ± 1.37	74.47 × 74.47 × 74.47	6168.88 ± 130.34	26262.25 ± 122.76	32431.12 ± 178.45
S7_2	0.97	293.08 ± 1.39	74.47 × 74.47 × 74.47	6180.58 ± 133.26	26273.33 ± 124.21	32453.91 ± 184.24
S7_3	0.97	293.06 ± 1.38	74.44 × 74.43 × 74.43	6131.71 ± 129.85	26271.70 ± 124.08	32403.41 ± 178.55
S7_4	0.96	293.00 ± 1.38	74.51 × 74.51 × 74.51	6243.62 ± 134.64	26278.46 ± 126.00	32522.08 ± 186.88
S7_5	0.97	293.01 ± 1.37	74.46 × 74.46 × 74.46	6170.99 ± 131.48	26266.62 ± 123.25	32437.61 ± 180.03
S8_1	0.97	293.03 ± 1.35	75.46 × 75.46 × 75.46	5197.16 ± 135.28	27357.40 ± 126.00	32554.57 ± 185.60
S8_2	0.96	293.00 ± 1.32	75.56 × 75.56 × 75.56	5320.10 ± 132.64	27354.39 ± 123.38	32674.50 ± 176.72
S8_3	0.97	293.09 ± 1.34	75.45 × 75.46 × 75.45	5211.16 ± 134.37	27362.61 ± 125.50	32573.76 ± 182.78
S8_4	0.97	293.12 ± 1.36	75.47 × 75.47 × 75.47	5197.57 ± 133.87	27365.91 ± 126.59	32563.48 ± 184.48
S8_5	0.97	293.05 ± 1.35	75.45 × 75.45 × 75.45	5152.40 ± 133.41	27359.54 ± 126.34	32511.94 ± 183.60
S9_1	0.96	293.04 ± 1.25	81.06 × 81.05 × 81.05	−110.21 ± 147.77	33643.59 ± 143.47	33533.38 ± 207.56
S9_2	0.96	293.10 ± 1.24	81.06 × 81.06 × 81.06	−94.79 ± 149.55	33650.79 ± 142.23	33556.00 ± 210.07
S9_3	0.96	293.06 ± 1.22	81.04 × 81.04 × 81.04	−125.76 ± 150.66	33646.74 ± 139.89	33520.98 ± 204.19
S9_4	0.96	293.07 ± 1.20	81.02 × 81.02 × 81.02	−145.72 ± 146-84	33647.86 ± 137.82	33502.14 ± 199.69
S9_5	0.96	293.08 ± 1.23	81.06 × 81.06 × 81.06	−126.51 ± 149.52	33648.56 ± 141.07	33522.05 ± 208.38

Table S10. Thermodynamic properties for the different MMA-systems studied.

System	ρ (g/cm³)	Temp. (K)	Volume (Å³)	Energies (kcal/mol)		
				E_{POT}	E_{KIN}	E_{TOT}
S10_1	0.97	293.06 ± 1.48	71.84 × 71.83 × 71.83	10804.33 ± 126.38	23640.49 ± 119.41	34444.82 ± 175.60
S10_2	0.97	293.05 ± 1.48	71.87 × 71.87 × 71.87	10846.69 ± 126.96	23639.49 ± 119.31	34486.19 ± 176.31
S10_3	0.97	293.08 ± 1.46	71.79 × 71.79 × 71.79	10759.66 ± 125.32	23642.16 ± 117.66	23642.16 ± 117.66
S10_4	0.97	293.15 ± 1.44	71.86 × 71.86 × 71.86	10844.68 ± 126.47	23647.56 ± 115.81	34492.24 ± 169.60
S10_5	0.97	293.10 ± 1.45	71.83 × 71.83 × 71.83	10799.07 ± 124.33	23643.54 ± 117.02	34442.61 ± 169.98
S11_1	0.97	293.10 ± 1.48	72.36 × 72.36 × 72.37	11013.07 ± 129.02	24102.84 ± 121.72	35115.91 ± 181.40
S11_2	0.97	293.06 ± 1.49	72.36 × 72.36 × 72.36	10978.22 ± 129.88	24099.48 ± 122.69	35077.69 ± 183.18
S11_3	0.97	293.12 ± 1.43	72.32 × 72.32 × 72.32	10943.41 ± 125.75	24100.12 ± 118.83	35043.52 ± 173.10
S11_4	0.97	292.97 ± 1.43	72.29 × 72.29 × 72.30	10918.09 ± 127.39	24092.73 ± 117.62	35010.82 ± 172.93
S11_5	0.97	293.16 ± 1.42	72.32 × 72.32 × 72.32	10952.41 ± 123.64	24107.92 ± 117.14	35060.33 ± 167.58
S12_1	0.97	293.11 ± 1.42	73.15 × 73.15 × 73.15	11168.88 ± 127.89	24944.17 ± 120.56	36113.05 ± 176.15
S12_2	0.97	293.07 ± 1.39	73.11 × 73.11 × 73.11	11120.21 ± 125.38	24940.93 ± 118.60	36061.14 ± 169.58
S12_3	0.97	293.04 ± 1.40	73.13 × 73.13 × 73.13	11134.02 ± 126.43	24938.35 ± 119.29	36072.38 ± 172.73
S12_4	0.96	293.06 ± 1.43	73.19 × 73.19 × 73.19	11187.90 ± 127.96	24939.72 ± 121.67	36127.62 ± 175.74
S12_5	0.97	293.04 ± 1.41	73.11 × 73.11 × 73.11	11109.28 ± 126.25	24938.20 ± 120.26	36047.49 ± 173.64
S13_1	0.96	293.11 ± 1.40	73.83 × 73.83 × 73.83	11352.42 ± 129.12	25622.85 ± 122.72	36975.27 ± 176.86
S13_2	0.96	293.13 ± 1.37	73.92 × 73.92 × 73.92	11456.76 ± 126.99	25625.30 ± 119.99	37082.06 ±171.76
S13_3	0.96	293.04 ± 1.39	73.87 × 73.87 × 73.87	11385.13 ± 127.29	25616.80 ± 121.35	37001.93 ± 174.46
S13_4	0.96	293.04 ± 1.39	73.94 × 73.94 × 73.94	11467.39 ± 130.60	25616.83 ± 121.76	37084.22 ± 178.40
S13_5	0.96	293.05 ± 1.40	73.87 × 73.87 × 73.87	11383.33 ± 132.18	25617.82 ± 122.40	37001.15 ± 180.95
S14_1	0.96	293.04 ± 1.32	75.95 × 75.95 × 75.95	11966.68 ± 132.19	27810.53 ± 125.65	39777.21 ± 179.64
S14_2	0.96	293.01 ± 1.32	75.86 × 75.86 × 75.86	11859.51 ± 133.00	27808.26 ± 125.67	39667.77 ± 180.42
S14_3	0.96	293.10 ± 1.35	76.03 × 76.03 × 76.03	12074.26 ± 137.51	27816.03 ± 128.55	39890.28 ± 190.68
S14_4	0.96	293.04 ± 1.34	76.00 × 76.01 × 76.01	12031.48 ± 134.04	27810.67 ± 126.74	39842.15 ± 183.60
S14_5	0.96	293.11 ± 1.36	75.96 × 75.96 × 75.96	11988.30 ± 135.15	27817.25 ± 128.81	39805.55 ± 188.40
S15_1	0.95	293.08 ± 1.20	81.92 × 81.92 × 81.92	13993.43 ± 149.36	34590.41 ± 141.93	48583.84 ± 205.85
S15_2	0.95	293.08 ± 1.20	81.92 × 81.91 × 81.92	13998.98 ± 149.10	34589.85 ± 141.64	48588.83 ± 204.97
S15_3	0.95	293.05 ± 1.20	81.92 × 81.92 × 81.92	13985.47 ± 147.74	34587.05 ± 141.24	48572.52 ± 202.46
S15_4	0.94	292.98 ± 1.21	81.94 × 81.93 × 81.94	13998.14 ± 148.18	34578.44 ± 142.39	48576.58 ± 205.46
S15_5	0.94	293.10 ± 1.20	81.94 × 81.94 × 81.95	14048.59 ± 148.23	34593.08 ± 141.80	48641.67 ± 204.48

Hydrogen Bond Analyses

Table S11. Summary of hydrogen bond events observed in the simulated MAA-MIP pre-polymerization mixtures. Values [a] are presented as averaged percent of total simulation time (% occupancy) per bupivacaine molecule with average lifetimes [b] and associated standard error of the mean (SEM).

System	Bupivacaine-MAA			
	O-HAA	N-HAA	HAB-OAD	HAB-OAC
S1_1	0.21 [6.50]	-	-	-
S1_2	0.35 [5.55 ± 2.21]	3.88 [2.80]	0.22 [1.10 ± 0.01]	-
S1_3	-	2.21 [2.60]	-	-
S1_4	-	-	0.01 [0.60]	-
S1_5	-	5.15 [3.20]	-	-

Table S11. *Cont.*

System	Bupivacaine-MAA			
	O-HAA	N-HAA	HAB-OAD	HAB-OAC
S2_1	3.37 [13.85 ± 23.20]	0.60 [1.60]	0.02 [0.65 ± 0.03]	-
S2_2	4.44 [7.30 ± 0.23]	0.55 [1.70]	-	-
S2_3	4.03 [5.47 ± 5.15]	1.15 [1.70 ± 0.25]	2.46 [0.90 ± 0.03]	0.03 [0.55 ± 0.00]
S2_4	27.74 [6.00 ± 2.42]	1.60 [1.90]	1.25 [0.98 ± 0.06]	0.02 [0.85 ± 0.03]
S2_5	10.09 [4.07 ± 4.11]	5.45 [2.37 ± 0.01]	1.05 [0.83 ± 0.05]	0.03 [0.60]
S3_1	12.68 [6.47 ± 15.42]	1.48 [2.80]	-	-
S3_2	5.05 [7.36 ± 6.22]	10.64 [2.85 ± 0.00]	2.71 [0.96 ± 0.03]	0.08 [0.58 ± 0.00]
S3_3	10.56 [7.31 ± 3.93]	3.24 [1.75 ± 0.63]	0.93 [0.74 ± 0.04]	0.02 [0.70 ± 0.01]
S3_4	17.52 [8.38 ± 0.67]	7.62 [2.12 ± 0.67]	2.07 [0.90 ± 0.03]	0.02 [0.53 ± 0.00]
S3_5	5.02 [5.62 ± 8.46]	0.00 [0.80]	-	-
S4_1	23.70 [7.72 ± 5.26]	14.27 [2.90 ± 0.07]	6.70 [1.10 ± 0.02]	0.15 [0.70 ± 0.01]
S4_2	5.31 [5.20 ± 3.70]	2.35 [1.67 ± 0.60]	0.62 [0.90 ± 0.02]	0.02 [0.57 ± 0.00]
S4_3	14.40 [6.74 ± 4.96]	7.36 [2.20 ± 0.29]	1.33 [0.94 ± 0.01]	0.02 [0.60 ± 0.02]
S4_4	17.36 [6.22 ± 3.61]	2.05 [2.40 ± 0.21]	4.58 [1.03 ± 0.03]	0.17 [0.64 ± 0.00]
S4_5	9.57 [7.46 ± 4.56]	2.84 [1.98 ± 0.55]	1.21 [1.07 ± 0.06]	0.00 [0.53 ± 0.00]
S5_1	23.67 [6.57 ± 2.97]	6.53 [1.95 ± 0.30]	1.93 [0.91 ± 0.04]	0.06 [0.65 ± 0.01]
S5_2	21.55 [8.01 ± 2.37]	8.54 [2.48 ± 0.03]	3.43 [0.95 ± 0.03]	0.06 [0.66 ± 0.01]
S5_3	15.51 [7.83 ± 1.32]	9.46 [2.48 ± 0.27]	1.19 [0.82 ± 0.05]	0.04 [0.60 ± 0.00]
S5_4	42.78 [7.93 ± 1.88]	17.91 [2.60 ± 0.06]	7.51 [1.07 ± 0.03]	0.05 [0.53 ± 0.00]
S5_5	39.44 [5.02 ± 2.44]	8.89 [2.38 ± 0.05]	2.38 [1.03 ± 0.03]	0.02 [0.53 ± 0.00]
S6_1	8.63 [4.82 ± 6.72]	10.03 [2.30 ± 0.08]	4.15 [0.93 ± 0.05]	0.02 [0.56 ± 0.00]
S6_2	19.83 [5.68 ± 3.31]	16.49 [2.43 ± 0.12]	8.48 [1.13 ± 0.05]	0.14 [0.37 ± 0.00]
S6_3	7.99 [5.27 ± 4.04]	13.15 [2.54 ± 0.15]	1.91 [0.89 ± 0.03]	0.05 [0.62 ± 0.02]
S6_4	20.15 [6.69 ± 3.33]	8.58 [2.68 ± 0.02]	2.58 [0.79 ± 0.03]	0.03 [0.60 ± 0.00]
S6_5	16.72 [5.88 ± 7.12]	6.92 [1.92 ± 0.24]	3.57 [1.07 ± 0.01]	0.07 [0.59 ± 0.01]
S7_1	11.07 [6.01 ± 3.66]	19.08 [2.30 ± 0.22]	3.20 [0.88 ± 0.04]	0.03 [0.62 ± 0.01]
S7_2	23.80 [3.94 ± 3.16]	5.02 [2.17 ± 0.31]	0.42 [0.72 ± 0.02]	0.01 [0.53 ± 0.00]
S7_3	12.35 [4.64 ± 4.07]	12.64 [2.20 ± 0.20]	5.70 [0.97 ± 0.04]	0.13 [0.69 ± 0.01]
S7_4	11.91 [5.89 ± 1.75]	11.56 [2.36 ± 0.04]	2.53 [1.08 ± 0.01]	0.08 [0.65 ± 0.00]
S7_5	16.54 [6.53 ± 3.97]	16.02 [2.26 ± 0.34]	6.72 [1.06 ± 0.02]	0.19 [0.59 ± 0.00]
S8_1	15.79 [6.61 ± 1.83]	10.35 [2.57 ± 0.00]	0.54 [0.67 ± 0.02]	0.01 [0.50 ± 0.00]
S8_2	26.42 [5.60 ± 3.74]	8.91 [1.47 ± 0.39]	1.44 [0.92 ± 0.04]	0.09 [0.58 ± 0.00]
S8_3	25.51 [7.91 ± 2.30]	8.40 [2.52 ± 0.06]	1.97 [0.95 ± 0.05]	0.16 [0.72 ± 0.01]
S8_4	31.15 [7.02 ± 3.31]	7.28 [1.87 ± 0.82]	2.70 [1.07 ± 0.03]	0.03 [0.53 ± 0.00]
S8_5	26.53 [6.36 ± 3.19]	13.08 [2.17 ± 0.26]	0.24 [0.90 ± 0.06]	0.02 [0.57 ± 0.00]
S9_1	43.09 [4.88 ± 2.49]	25.58 [2.46 ± 0.11]	10.99 [1.06 ± 0.02]	0.27 [0.67 ± 0.00]
S9_2	36.46 [8.46 ± 0.91]	34.40 [8.46 ± 0.91]	14.35 [1.10 ± 0.02]	0.27 [0.64 ± 0.01]
S9_3	32.85 [5.63 ± 2.17]	24.02 [2.05 ± 0.17]	13.39 [1.12 ± 0.02]	0.21 [0.55 ± 0.00]
S9_4	45.30 [5.30 ± 2.83]	24.09 [2.18 ± 0.21]	12.41 [0.94 ± 0.02]	0.29 [0.64 ± 0.00]
S9_5	35.75 [6.31 ± 3.24]	20.99 [2.23 ± 0.13]	7.56 [1.00 ± 0.02]	0.39 [0.64 ± 0.00]

Table S11. *Cont.*

System	Bupivacaine-EGDMA			
	HAB-OAE	HAB-OAF	HAB-OAI	HAB-OAJ
S0_1	16.99 [1.05 ± 0.04]	24.62 [1.27 ± 0.04]	0.00 [0.50]	0.01 [0.65 ± 0.03]
S0_2	16.54 [1.11 ± 0.04]	31.29 [1.22 ± 0.02]	0.00 [0.62 ± 0.03]	0.00 [0.50 ± 0.00]
S0_3	22.98 [1.06 ± 0.03]	20.72 [1.05 ± 0.03]	0.01 [0.60 ± 0.02]	0.02 [0.54 ± 0.04]
S0_4	18.51 [1.21 ± 0.03]	22.83 [1.23 ± 0.03]	0.03 [0.55 ± 0.00]	0.01 [0.53 ± 0.00]
S0_5	17.97 [1.22 ± 0.03]	26.64 [1.25 ± 0.03]	0.01 [0.55 ± 0.00]	0.00 [0.55 ± 0.00]
S1_1	26.30 [1.09 ± 0.04]	17.78 [1.26 ± 0.03]	0.00 [0.50]	0.01 [0.52 ± 0.00]
S1_2	15.04 [1.29 ± 0.03]	27.99 [1.25 ± 0.03]	0.01 [0.50 ± 0.00]	0.05 [0.62 ± 0.01]
S1_3	11.24 [0.98 ± 0.04]	31.15 [1.18 ± 0.04]	0.01 [0.60]	0.05 [0.52 ± 0.00]
S1_4	23.54 [1.14 ± 0.03]	14.58 [1.22 ± 0.02]	0.00 [0.73 ± 0.04]	0.00 [0.60 ± 0.02]
S1_5	21.08 [1.05 ± 0.04]	21.67 [1.14 ± 0.05]	0.01 [0.83 ± 0.05]	0.00 [0.50 ± 0.00]
S2_1	24.66 [1.18 ± 0.02]	14.78 [1.10 ± 0.04]	0.01 [0.53 ± 0.00]	0.00 [0.55 ± 0.00]
S2_2	11.92 [1.15 ± 0.04]	32.22 [1.15 ± 0.03]	0.03 [0.57 ± 0.00]	0.01 [0.50 ± 0.00]
S2_3	19.31 [1.07 ± 0.05]	11.25 [1.05 ± 0.04]	0.01 [0.53 ± 0.00]	-
S2_4	12.62 [0.96 ± 0.05]	19.96 [1.08 ± 0.04]	0.01 [0.57 ± 0.01]	0.03 [0.70 ± 0.01]
S2_5	14.07 [1.11 ± 0.04]	26.72 [1.23 ± 0.04]	0.00 [0.60 ± 0.01]	0.01 [0.58 ± 0.01]
S3_1	15.27 [1.13 ± 0.04]	23.96 [1.25 ± 0.03]	0.04 [0.05 ± 0.00]	0.00 [0.50 ± 0.00]
S3_2	21.35 [1.24 ± 0.05]	26.59 [1.27 ± 0.04]	0.00 [0.60 ± 0.02]	0.00 [0.60]
S3_3	14.86 [1.27 ± 0.03]	22.90 [1.32 ± 0.04]	0.01 [0.60 ± 0.01]	0.02 [0.70 ± 0.04]
S3_4	17.41 [1.07 ± 0.05]	17.87 [1.08 ± 0.03]	0.01 [0.75 ± 0.09]	0.00 [0.60 ± 0.02]
S3_5	18.50 [1.23 ± 0.03]	28.77 [1.30 ± 0.02]	0.03 [0.53 ± 0.00]	0.00 [0.55 ± 0.00]
S4_1	19.67 [1.20 ± 0.03]	23.54 [1.31 ± 0.03]	0.02 [0.55 ± 0.00]	0.07 [0.57 ± 0.01]
S4_2	18.55 [1.11 ± 0.03]	14.95 [1.14 ± 0.03]	0.01 [0.72 ± 0.05]	0.00 [0.50 ± 0.00]
S4_3	22.78 [1.25 ± 0.03]	19.32 [1.07 ± 0.03]	0.00 [1.00 ± 0.35]	0.04 [0.51 ± 0.00]
S4_4	11.92 [1.06 ± 0.03]	16.76 [1.10 ± 0.03]	0.01 [0.60 ± 0.00]	0.02 [0.53 ± 0.00]
S4_5	25.33 [1.29 ± 0.04]	17.50 [1.21 ± 0.03]	0.01 [0.50 ± 0.00]	0.01 [0.55 ± 0.00]
S5_1	11.90 [1.01 ± 0.03]	13.92 [1.10 ± 0.04]	0.00 [0.50 ± 0.00]	0.01 [0.01 ± 0.01]
S5_2	16.40 [1.05 ± 0.03]	19.33 [1.23 ± 0.03]	0.00 [0.50]	0.01 [0.87 ± 0.03]
S5_3	16.37 [1.11 ± 0.03]	16.02 [1.00 ± 0.03]	0.01 [0.50 ± 0.00]	0.01 [0.50 ± 0.00]
S5_4	22.51 [1.25 ± 0.05]	16.84 [1.24 ± 0.04]	0.02 [0.53 ± 0.00]	0.00 [0.50 ± 0.00]
S5_5	23.35 [1.18 ± 0.03]	14.45 [1.28 ± 0.06]	0.00 [0.75 ± 0.00]	0.00 [0.55 ± 0.00]
S6_1	19.17 [1.09 ± 0.03]	16.17 [1.28 ± 0.02]	0.05 [0.53 ± 0.00]	0.00 [0.50 ± 0.00]
S6 _2	17.19 [1.18 ± 0.04]	22.59 [1.27 ± 0.02]	0.01 [0.54 ± 0.00]	0.00 [0.52 ± 0.00]
S6_3	17.32 [1.21 ± 0.03]	22.13 [1.36 ± 0.05]	0.01 [0.53 ± 0.00]	0.01 [0.50 ± 0.00]
S6_4	17.67 [1.24 ± 0.05]	15.77 [1.22 ± 0.04]	0.02 [0.50 ± 0.00]	0.02 [0.52 ± 0.00]
S6_5	24.12 [1.21 ± 0.02]	11.73 [1.18 ± 0.03]	0.03 [0.54 ± 0.00]	0.03 [0.60 ± 0.01]
S7_1	14.40 [1.24 ± 0.03]	22.23 [1.22 ± 0.03]	0.01 [0.53 ± 0.00]	0.00 [0.50 ± 0.00]
S7_2	19.77 [1.21 ± 0.03]	12.08 [1.21 ± 0.04]	0.04 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S7_3	17.13 [1.08 ± 0.04]	15.27 [1.03 ± 0.03]	0.00 [0.65 ± 0.03]	0.00 [0.60]
S7_4	16.76 [1.23 ± 0.04]	16.20 [1.11 ± 0.03]	0.01 [0.57 ± 0.01]	0.03 [0.53 ± 0.00]
S7_5	28.40 [1.24 ± 0.03]	9.22 [1.13 ± 0.03]	0.01 [0.51 ± 0.00]	0.01 [0.53 ± 0.00]
S8_1	16.30 [1.10 ± 0.04]	17.31 [1.10 ± 0.04]	0.00 [0.53 ± 0.00]	0.01 [0.50 ± 0.00]
S8_2	12.77 [1.04 ± 0.05]	22.85 [1.19 ± 0.03]	0.00 [0.50]	0.00 [0.50 ± 0.00]
S8_3	17.42 [1.19 ± 0.02]	23.46 [1.19 ± 0.03]	0.04 [0.63 ± 0.01]	0.04 [0.54 ± 0.00]
S8_4	24.43 [1.16 ± 0.03]	16.01 [1.10 ± 0.04]	0.00 [0.60 ± 0.02]	0.01 [0.52 ± 0.00]
S8_5	16.35 [1.15 ± 0.04]	19.83 [1.20 ± 0.05]	0.01 [0.11 ± 0.01]	0.00 [0.09 ± 0.02]

Table S11. *Cont.*

System	Bupivacaine-EGDMA			
	HAB-OAE	HAB-OAF	HAB-OAI	HAB-OAJ
S9_1	14.18 [1.12 ± 0.05]	9.96 [1.40 ± 0.08]	0.02 [0.50 ± 0.00]	0.00 [0.65 ± 0.03]
S9_2	9.96 [1.17 ± 0.05]	7.39 [1.10 ± 0.08]	0.01 [0.65 ± 0.03]	0.01 [0.53 ± 0.00]
S9_3	6.72 [1.22 ± 0.12]	12.26 [1.22 ± 0.01]	0.30 [0.50 ± 0.00]	0.01 [0.55 ± 0.00]
S9_4	11.64 [1.21 ± 0.09]	11.71 [1.19 ± 0.04]	0.00 [0.65 ± 0.03]	0.01 [0.62 ± 0.03]
S9_5	10.77 [1.06 ± 0.04]	22.96 [1.27 ± 0.03]	0.01 [0.65 ± 0.03]	0.00 [0.50 ± 0.00]
System	**Bupivacaine-Bupivacaine**			
	O-HAB	**N-HAB**		
S0_1	-	-		
S0_2	2.50 [2.20]	-		
S0_3	-	-		
S0_4	-	-		
S0_5	-	-		
S1_1	-	-		
S1_2	-	-		
S1_3	-	-		
S1_4	0.56 [1.90]	-		
S1_5	-	-		
S2 _1	-	-		
S2_2	-	-		
S2_3	-	-		
S2_4	-	-		
S2_5	-	-		
S3_1	2.83 [2.20]	-		
S3_2	3.41 [2.10]	-		
S3_3	-	-		
S3_4	-	-		
S3_5	-	-		
S4_1	-	-		
S4_2	-	-		
S4_3	-	-		
S4_4	4.39 [2.20]	-		
S4_5	-	-		
S5_1	7.57 [2.40]	-		
S5_2	4.89 [2.20]	-		
S5_3	-	-		
S5_4	-	-		
S5_5	-	-		

[a] The data obtained for a specific interaction point analyzed in a simulated system were added together and then divided by the number of analyzed molecules in that system resulting in an average percentage (% occupancy) of the total production time that an interaction point is engaged in hydrogen bonding. [b] Average lifetimes were calculated by summarizing all lifetimes corresponding to formed hydrogen bonds at an analyzed interaction point in a simulated system and then divided by the number of hydrogen bond events in that system. Values are presented as [average lifetimes ± SEM]. For single events no SEM was calculated. See Figure 1 for denotation of the atoms.

Table S12. Summary of hydrogen bond events observed in the simulated MMA-MIP pre-polymerization mixtures. Values [a] are presented as averaged percent of total simulation time (% occupancy) per bupivacaine molecule with average lifetimes [b] and associated standard error of the mean.

System	Bupivacaine-MMA	
	OAD-HAB	**OAE-HAB**
S10_1	4.54 [1.10 ± 0.06]	0.00 [0.50]
S10_2	4.05 [1.16 ± 0.09]	0.00 [0.50]
S10_3	5.28 [1.05 ± 0.03]	0.00 [0.50]
S10_4	4.67 [0.81 ± 0.06]	0.00 [0.70]
S10_5	3.23 [0.90 ± 0.07]	0.00 [0.50]
S11_1	3.66 [1.07 ± 0.08]	-
S11_2	1.65 [1.40 ± 0.01]	0.00 [0.50]
S11_3	5.78 [0.94 ± 0.04]	0.00 [0.55 ± 0.00]
S11_4	8.65 [1.20 ± 0.05]	0.00 [0.50 ± 0.00]
S11_5	2.28 [1.42 ± 0.02]	0.00 [0.50 ± 0.00]
S12_1	6.36 [1.18 ± 0.02]	0.00 [0.50 ± 0.00]
S12_2	4.83 [1.18 ± 0.02]	0.00 [0.50 ± 0.00]
S12_3	4.54 [1.33 ± 0.01]	0.00 [0.50 ± 0.00]
S12_4	1.46 [1.04 ± 0.10]	0.00 [0.50]
S12_5	4.39 [1.33 ± 0.01]	-
S13_1	8.34 [1.21 ± 0.03]	0.01 [0.50 ± 0.00]
S13_2	6.86 [1.09 ± 0.03]	0.01 [0.50 ± 0.00]
S13_3	2.98 [1.32 ± 0.01]	-
S13_4	8.63 [1.05 ± 0.04]	0.01 [0.55 ± 0.00]
S13_5	6.50 [1.04 ± 0.03]	0.02 [0.55 ± 0.00]
S14_1	10.02 [1.16 ± 0.03]	0.01 [0.60 ± 0.20]
S14_2	6.88 [1.14 ± 0.03]	0.00 [0.67 ± 0.05]
S14_3	4.02 [1.13 ± 0.02]	0.00 [0.53 ± 0.00]
S14_4	13.23 [1.21 ± 0.30]	0.00 [0.50]
S14_5	6.06 [1.09 ± 0.03]	0.00 [0.75 ± 0.09]
S15_1	9.17 [1.07 ± 0.03]	0.00 [0.50 ± 0.00]
S15_2	8.50 [0.88 ± 0.03]	0.01 [0.50]
S15_3	21.73 [1.13 ± 0.01]	0.01 [0.51 ± 0.00]
S15_4	13.60 [1.03 ± 0.02]	0.00 [0.50 ± 0.00]
S15_5	7.39 [0.96 ± 0.03]	0.01 [0.52 ± 0.00]

System	Bupivacaine-EGDMA			
	HAB-OAE	**HAB-OAF**	**HAB-OAI**	**HAB-OAJ**
S10_1	13.23 [1.11 ± 0.04]	16.00 [1.07 ± 0.04]	0.00 [0.50]	0.00 [0.50]
S10_2	18.87 [1.21 ± 0.04]	23.46 [1.27 ± 0.02]	-	0.02 [0.58 ± 0.01]
S10_3	24.20 [1.32 ± 0.01]	14.37 [1.35 ± 0.04]	0.00 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S10_4	24.43 [1.24 ± 0.01]	15.73 [1.26 ± 0.34]	0.01 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S10_5	22.23 [1.18 ± 0.03]	16.17 [1.05 ± 0.04]	0.01 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S11_1	17.53 [1.16 ± 0.03]	21.82 [1.21 ± 0.05]	0.02 [0.55 ± 0.00]	0.01 [0.50 ± 0.00]
S11_2	24.65 [1.37 ± 0.02]	22.11 [1.30 ± 0.02]	0.00 [0.55 ± 0.01]	0.01 [0.60]
S11_3	19.08 [1.17 ± 0.03]	17.33 [1.18 ± 0.03]	0.03 [0.58 ± 0.01]	0.02 [0.60 ± 0.01]
S11_4	18.80 [0.99 ± 0.04]	17.43 [1.13 ± 0.04]	0.00 [0.65 ± 0.03]	0.00 [0.60 ± 0.01]
S11_5	21.17 [1.27 ± 0.04]	25.10 [1.24 ± 0.02]	0.01 [0.73 ± 0.02]	0.01 [0.62 ± 0.02]

Table S12. *Cont.*

System	Bupivacaine-MMA			
	OAD-HAB	**OAE-HAB**	**-**	**-**
S12_1	18.23 [1.14 ± 0.03]	17.43 [1.17 ± 0.03]	0.03 [0.53 ± 0.00]	0.02 [0.56 ± 0.01]
S12_2	25.67 [1.30 ± 0.02]	19.43 [1.25 ± 0.02]	0.01 [0.50 ± 0.00]	0.02 [0.56 ± 0.01]
S12_3	16.17 [1.18 ± 0.03]	14.12 [1.15 ± 0.03]	0.01 [0.63 ± 0.01]	0.00 [0.63 ± 0.01]
S12_4	14.12 [1.15 ± 0.03]	29.15 [1.14 ± 0.02]	0.01 [0.52 ± 0.00]	0.00 [0.63 ± 0.01]
S12_5	21.49 [1.40 ± 0.03]	23.12 [1.28 ± 0.02]	0.01 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S13_1	19.78 [1.16 ± 0.03]	18.09 [1.13 ± 0.03]	0.02 [0.57 ± 0.01]	0.01 [0.53 ± 0.00]
S13_2	20.60 [1.17 ± 0.03]	15.17 [1.31 ± 0.05]	0.02 [0.62 ± 0.02]	0.02 [0.59 ± 0.01]
S13_3	22.16 [1.15 ± 0.03]	16.82 [1.17 ± 0.02]	0.00 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S13_4	12.78 [1.03 ± 0.04]	12.57 [0.94 ± 0.04]	0.02 [0.56 ± 0.00]	0.00 [0.50 ± 0.00]
S13_5	16.11 [1.02 ± 0.04]	13.78 [1.05 ± 0.04]	0.03 [0.51 ± 0.00]	0.01 [0.57 ± 0.00]
S14_1	11.65 [1.08 ± 0.04]	12.39 [1.07 ± 0.03]	0.02 [0.52 ± 0.00]	0.00 [0.65 ± 0.03]
S14_2	15.40 [1.30 ± 0.03]	21.90 [1.27 ± 0.05]	0.03 [0.65 ± 0.03]	0.01 [0.63 ± 0.01]
S14_3	25.66 [1.11 ± 0.02]	9.35 [1.09 ± 0.04]	0.02 [0.56 ± 0.01]	0.05 [0.65 ± 0.00]
S14_4	24.44 [1.35 ± 0.02]	11.19 [1.17 ± 0.03]	0.01 [0.57 ± 0.01]	0.03 [0.57 ± 0.00]
S14_5	12.30 [1.19 ± 0.02]	19.44 [1.26 ± 0.01]	0.03 [0.61 ± 0.02]	0.02 [0.53 ± 0.00]
S15_1	19.15 [1.29 ± 0.06]	12.95 [1.15 ± 0.05]	0.05 [0.65 ± 0.00]	0.01 [0.50 ± 0.00]
S15_2	14.42 [1.03 ± 0.03]	13.78 [1.12 ± 0.03]	0.01 [0.50 ± 0.00]	0.00 [0.50 ± 0.00]
S15_3	9.82 [1.15 ± 0.03]	10.77 [1.19 ± 0.03]	0.00 [0.50 ± 0.00]	0.01 [0.60 ± 0.01]
S15_4	19.18 [1.19 ± 0.03]	11.21 [1.32 ± 0.06]	0.01 [0.53 ± 0.00]	0.59 [0.53 ± 0.00]
S15_5	17.72 [1.17 ± 0.06]	7.03 [1.12 ± 0.04]	0.29 [0.55 ± 0.01]	0.00 [0.50]

System	Bupivacaine-Bupivacaine	
	O-HAB	**N-HAB**
S11_1	-	-
S11_2	-	-
S11_3	-	-
S11_4	0.01 [0.50]	-
S11_5	-	-
S15_1		-
S15_2	0.05 [0.50]	-
S15_3	-	-
S15_4		-
S15_5	6.37 [2.00]	-

[a] The data obtained for a specific interaction point analyzed in a simulated system were added together and then divided by the number of analyzed molecules in that system resulting in an average percentage (% occupancy) of the total production time that an interaction point is engaged in hydrogen bonding. [b] Average lifetimes were calculated by summarizing all lifetimes corresponding to formed hydrogen bonds at an analyzed interaction point in a simulated system and then divided by the number of hydrogen bond events in that system. Values are presented as [average lifetimes ± SEM]. For single events no SEM was calculated. See Figure 1 for denotation of the atoms.

PCA Residual Variance Plot

Figure S1. The residual variance plot of the PCA on data obtained from rebinding studies, surface characterization and MD simulation trajectories.