Supporting Table 1

Non-bond potential

Bead i	Bead j	$\sigma_{i,j}$ (nm)	ε (kJ/mol)	Bead i	Bead j	$\sigma_{i,j}$ (nm)	ε (kJ/mol)	Bead i	Bead j	$\sigma_{i,j}$ (nm)	ε (kJ/mol)
Bead1	Bead1	0.394	0.929	Bead3(2)	Bead7	0.495	2.197	Bead3(7)	Bead9	0.457	1.957
Bead1	Bead2	0.404	0.959	Bead3(2)	Bead8	0.480	2.271	Bead3(7)	Bead7	0.485	2.165
Bead1	Bead3(1)	0.466	1.613	Bead3(2)	Bead10	0.495	2.876	Bead3(7)	Bead8	0.470	2.304
Bead1	Bead3(2)	0.486	1.768	Bead3(2)	Bead11	0.480	2.109	Bead3(7)	Bead10	0.495	2.891
Bead1	Bead3(3)	0.446	1.443	Bead3(2)	Bead12	0.495	2.114	Bead3(7)	Bead11	0.460	2.091
Bead1	Bead3(4)	0.456	1.687	Bead3(2)	Bead13	0.495	1.414	Bead3(7)	Bead12	0.495	2.157
Bead1	Bead3(5)	0.466	1.566	Bead3(3)	Bead3(3)	0.439	5.772	Bead3(7)	Bead13	0.475	1.365
Bead1	Bead3(6)	0.486	1.846	Bead3(3)	Bead3(4)	0.479	5.815	Bead4	Bead4	0.462	2.164
Bead1	Bead3(7)	0.466	1.745	Bead3(3)	Bead3(5)	0.459	5.668	Bead4	Bead5	0.435	1.499
Bead1	Bead4	0.438	1.366	Bead3(3)	Bead3(6)	0.489	5.642	Bead4	Bead6	0.443	2.753
Bead1	Bead5	0.411	1.018	Bead3(3)	Bead3(7)	0.479	5.777	Bead4	Bead9	0.428	1.431
Bead1	Bead6	0.429	1.713	Bead3(3)	Bead4	0.460	2.924	Bead4	Bead7	0.456	1.647
Bead1	Bead9	0.394	1.038	Bead3(3)	Bead5	0.444	1.621	Bead4	Bead8	0.442	1.643
Bead1	Bead7	0.412	1.202	Bead3(3)	Bead6	0.421	4.319	Bead4	Bead10	0.466	2.052
Bead1	Bead8	0.398	1.110	Bead3(3)	Bead9	0.437	1.582	Bead4	Bead11	0.431	1.599
Bead1	Bead10	0.432	1.313	Bead3(3)	Bead7	0.445	1.759	Bead4	Bead12	0.456	1.656
Bead1	Bead11	0.397	1.112	Bead3(3)	Bead8	0.430	1.916	Bead4	Bead13	0.446	1.166
Bead1	Bead12	0.412	1.106	Bead3(3)	Bead10	0.465	2.529	Bead5	Bead5	0.409	1.085
Bead1	Bead13	0.392	0.885	Bead3(3)	Bead11	0.430	1.850	Bead5	Bead6	0.426	1.833
Bead2	Bead2	0.394	0.927	Bead3(3)	Bead12	0.475	1.789	Bead5	Bead9	0.402	1.113
Bead2	Bead3(1)	0.466	1.648	Bead3(3)	Bead13	0.455	1.164	Bead5	Bead7	0.420	1.235
Bead2	Bead3(2)	0.476	1.755	Bead3(4)	Bead3(4)	0.489	5.981	Bead5	Bead8	0.405	1.201
Bead2	Bead3(3)	0.446	1.419	Bead3(4)	Bead3(5)	0.479	5.898	Bead5	Bead10	0.440	1.429
Bead2	Bead3(4)	0.456	1.648	Bead3(4)	Bead3(6)	0.509	5.869	Bead5	Bead11	0.395	1.174
Bead2	Bead3(5)	0.466	1.578	Bead3(4)	Bead3(7)	0.499	6.109	Bead5	Bead12	0.420	1.176
Bead2	Bead3(6)	0.486	1.836	Bead3(4)	Bead4	0.480	3.168	Bead5	Bead13	0.390	0.929
Bead2	Bead3(7)	0.466	1.660	Bead3(4)	Bead5	0.464	2.007	Bead6	Bead6	0.394	3.429
Bead2	Bead4	0.438	1.329	Bead3(4)	Bead6	0.451	4.337	Bead6	Bead9	0.429	1.809
Bead2	Bead5	0.401	1.010	Bead3(4)	Bead9	0.447	1.808	Bead6	Bead7	0.447	2.069
Bead2	Bead6	0.429	1.753	Bead3(4)	Bead7	0.475	2.207	Bead6	Bead8	0.423	2.088
Bead2	Bead9	0.384	0.994	Bead3(4)	Bead8	0.460	2.259	Bead6	Bead10	0.437	2.511
Bead2	Bead7	0.422	1.142	Bead3(4)	Bead10	0.495	2.929	Bead6	Bead11	0.412	1.995
Bead2	Bead8	0.398	1.128	Bead3(4)	Bead11	0.450	2.117	Bead6	Bead12	0.437	1.996
Bead2	Bead10	0.442	1.335	Bead3(4)	Bead12	0.475	2.148	Bead6	Bead13	0.437	1.558
Bead2	Bead11	0.387	1.095	Bead3(4)	Bead13	0.475	1.372	Bead7	Bead7	0.430	1.400
Bead2	Bead12	0.422	1.126	Bead3(5)	Bead3(5)	0.459	5.648	Bead7	Bead8	0.426	1.378
Bead2	Bead13	0.392	0.864	Bead3(5)	Bead3(6)	0.509	5.493	Bead7	Bead10	0.450	1.638
Bead3(1)	Bead3(1)	0.489	5.570	Bead3(5)	Bead3(7)	0.499	5.813	Bead7	Bead11	0.415	1.328
Bead3(1)	Bead3(2)	0.489	5.370	Bead3(5)	Bead4	0.480	3.111	Bead7	Bead12	0.430	1.356
Bead3(1)	Bead3(3)	0.469	5.583	Bead3(5)	Bead5	0.464	1.828	Bead7	Bead13	0.410	1.077
Bead3(1)	Bead3(4)	0.479	5.705	Bead3(5)	Bead6	0.451	4.274	Bead8	Bead8	0.412	1.317
Bead3(1)	Bead3(5)	0.489	5.570	Bead3(5)	Bead9	0.447	1.841	Bead8	Bead10	0.436	1.607
Bead3(1)	Bead3(6)	0.519	5.460	Bead3(5)	Bead7	0.485	2.118	Bead8	Bead11	0.401	1.310
Bead3(1)	Bead3(7)	0.499	5.656	Bead3(5)	Bead8	0.460	2.063	Bead8	Bead12	0.426	1.313
Bead3(1)	Bead4	0.480	3.001	Bead3(5)	Bead10	0.475	2.878	Bead8	Bead13	0.406	1.035
Bead3(1)	Bead5	0.464	1.837	Bead3(5)	Bead11	0.450	1.967	Bead9	Bead9	0.385	1.100
Bead3(1)	Bead6	0.441	4.114	Bead3(5)	Bead12	0.475	2.033	Bead9	Bead7	0.402	1.219
Bead3(1)	Bead9	0.467	1.756	Bead3(5)	Bead13	0.465	1.322	Bead9	Bead8	0.398	1.202
Bead3(1)	Bead7	0.485	2.051	Bead3(6)	Bead3(6)	0.539	5.449	Bead9	Bead10	0.423	1.462
Bead3(1)	Bead8	0.460	2.090	Bead3(6)	Bead3(7)	0.529	5.728	Bead9	Bead11	0.387	1.203
Bead3(1)	Bead10	0.485	2.749	Bead3(6)	Bead4	0.510	3.186	Bead9	Bead12	0.412	1.228
Bead3(1)	Bead11	0.460	1.907	Bead3(6)	Bead5	0.494	2.102	Bead9	Bead13	0.392	0.950
Bead3(1)	Bead12	0.475	2.013	Bead3(6)	Bead6	0.461	4.287	Bead10	Bead10	0.471	1.984
Bead3(1)	Bead13	0.475	1.318	Bead3(6)	Bead9	0.477	2.041	Bead10	Bead11	0.436	1.605
Bead3(2)	Bead3(2)	0.499	5.298	Bead3(6)	Bead7	0.495	2.325	Bead10	Bead12	0.450	1.581
Bead3(2)	Bead3(3)	0.479	5.655	Bead3(6)	Bead8	0.490	2.305	Bead10	Bead13	0.431	1.267
Bead3(2)	Bead3(4)	0.489	5.565	Bead3(6)	Bead10	0.515	2.952	Bead11	Bead11	0.390	1.287
Bead3(2)	Bead3(5)	0.489	5.582	Bead3(6)	Bead11	0.480	2.167	Bead11	Bead12	0.415	1.286
Bead3(2)	Bead3(6)	0.529	5.529	Bead3(6)	Bead12	0.505	2.280	Bead11	Bead13	0.385	1.062
Bead3(2)	Bead3(7)	0.499	5.492	Bead3(6)	Bead13	0.495	1.617	Bead12	Bead12	0.440	1.328
Bead3(2)	Bead4	0.490	3.105	Bead3(7)	Bead3(7)	0.509	6.031	Bead12	Bead13	0.410	1.051
Bead3(2)	Bead5	0.484	1.985	Bead3(7)	Bead4	0.490	3.232	Bead13	Bead13	0.390	0.861
Bead3(2)	Bead6	0.471	4.203	Bead3(7)	Bead5	0.474	1.957				
Bead3(2)	Bead9	0.487	1.966	Bead3(7)	Bead6	0.451	4.382				

Supporting Table 2

Bond Potential

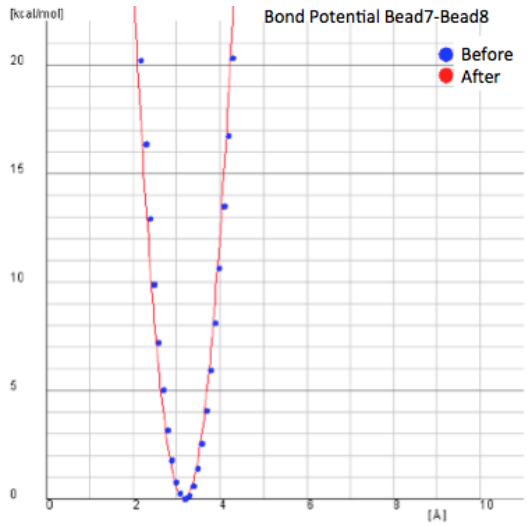
Bond Pair	R_0 (nm)	K(kJ/mol·nm^2)
Bead2-Bead1	0.198	151.993
Bead2-Bead3(1)	0.337	20.707
Bead3(1)-Bead3(2)	0.703	6.397
Bead3(2)-Bead3(3)	0.604	5.785
Bead3(3)-Bead3(4)	0.802	2.809
Bead3(4)-Bead3(5)	0.455	1.846
Bead3(6)-Bead3(5)	0.465	1.891
Bead3(6)-Bead3(7)	0.426	0.505
Bead3(7)-Bead4	0.564	15.295
Bead4-Bead5	0.317	110.365
Bead5-Bead6	0.277	14.652
Bead6-Bead7	0.406	79.958
Bead7-Bead10	0.337	153.827
Bead7-Bead8	0.317	147.752
Bead7-Bead9	0.327	154.103
Bead10-Bead11	0.238	57.256
Bead11-Bead12	0.238	143.230
Bead13-Bead12	0.208	157.087
Bead13-Bead13	0.350	154.864

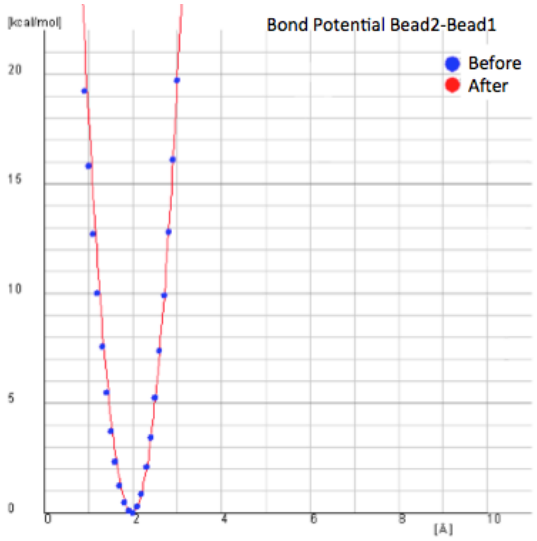
Angle Potential

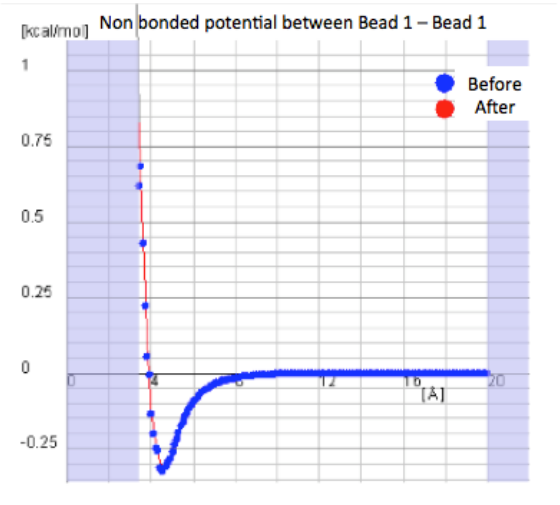
Angle Pair	θ_0 (rad)	K(kJ/mol)
Bead1-Bead2-Bead3(1)	57.680	311.094
Bead2-Bead1-Bead2	62.652	1188.069
Bead2-Bead3(1)-Bead3(2)	63.646	208.215
Bead3(1)-Bead3(2)-Bead3(3)	0.000	30.149
Bead3(2)-Bead3(3)-Bead3(4)	20.884	21.872
Bead3(3)-Bead3(4)-Bead3(5)	0.000	-4.026
Bead3(4)-Bead3(5)-Bead3(6)	8.950	-3.905
Bead3(6)-Bead3(7)-Bead4	18.895	64.308
Bead3(5)-Bead3(6)-Bead3(7)	5.967	3.328
Bead3(7)-Bead4-Bead5	15.912	40.600
Bead4-Bead5-Bead6	81.547	135.251
Bead5-Bead6-Bead7	96.464	71.240
Bead6-Bead7-Bead10	0.000	83.103
Bead6-Bead7-Bead9	109.392	645.531
Bead6-Bead7-Bead8	74.586	584.722
Bead7-Bead10-Bead11	87.514	278.180
Bead8-Bead7-Bead10	121.326	1072.882
Bead9-Bead7-Bead10	60.663	525.230
Bead8-Bead7-Bead9	4.972	1047.869
Bead10-Bead11-Bead12	52.707	179.061
Bead11-Bead12-Bead13	99.448	1688.580

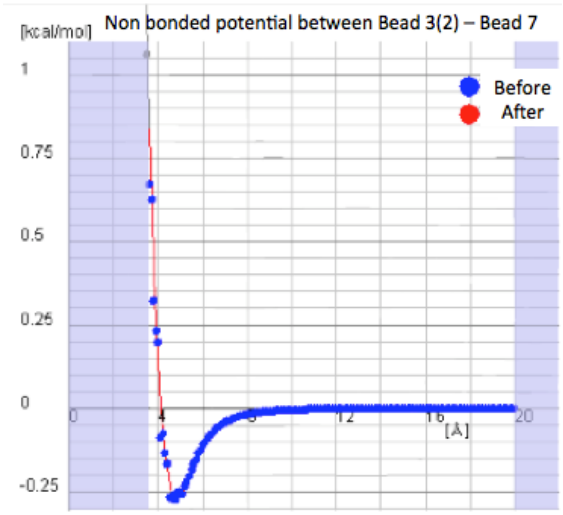
Torsion Potential

Tosrion Pair	a1(kJ/mol)	a2(kJ/mol)	a3(kJ/mol)	a4(kJ/mol)	a5(kJ/mol)
Bead1-Bead2-Bead3(1)-Bead3(2)	10.308	5.720	-0.409	-0.381	-2.975
Bead2-Bead1-Bead2-Bead3(1)	10.153	7.210	-2.306	-2.798	0.877
Bead2-Bead3(1)-Bead3(2)-Bead3(3)	4.127	6.854	3.225	-3.497	-1.041
Bead3(1)-Bead3(2)-Bead3(3)-Bead3(4)	3.065	-0.403	-3.246	-1.479	3.418
Bead3(2)-Bead3(3)-Bead3(4)-Bead3(5)	0.946	3.754	4.345	-2.917	0.136
Bead3(3)-Bead3(4)-Bead3(5)-Bead3(6)	6.395	1.559	-1.279	-1.038	-0.891
Bead3(4)-Bead3(5)-Bead3(6)-Bead3(7)	4.687	-1.245	-2.556	-1.357	1.620
Bead3(5)-Bead3(6)-Bead3(7)-Bead4	1.978	0.942	1.397	0.346	-1.975
Bead3(6)-Bead3(7)-Bead4-Bead5	2.299	-0.788	-1.473	0.476	-0.015
Bead3(7)-Bead4-Bead5-Bead6	6.671	-1.838	-6.508	2.649	3.362
Bead4-Bead5-Bead6-Bead7	5.443	5.279	2.010	-1.377	1.205
Bead5-Bead6-Bead7-Bead10	1.984	0.664	9.445	1.284	-7.473
Bead5-Bead6-Bead7-Bead8	3.582	3.073	3.062	-1.422	-1.444
Bead5-Bead6-Bead7-Bead9	3.375	-3.871	1.982	2.555	-0.256
Bead6-Bead7-Bead10-Bead11	3.387	1.660	3.374	-3.822	-3.838
Bead8-Bead7-Bead10-Bea11	2.917	-4.092	14.907	3.987	-5.060
Bead9-Bead7-Bead10-Bead11	3.180	2.732	14.177	-2.835	-4.625
Bead7-Bead10-Bead11-Bead12	5.651	-3.331	-2.135	3.498	1.292
Bead12-Bead13-Bead13-Bead12	14.533	0.454	-2.577	-5.700	-2.896
Bead10-Bead11-Bead12-Bead13	4.514	-1.489	1.947	-1.619	1.772
Bead11-Bead12-Bead13-Bead13	13.365	9.742	-12.853	-9.493	14.048

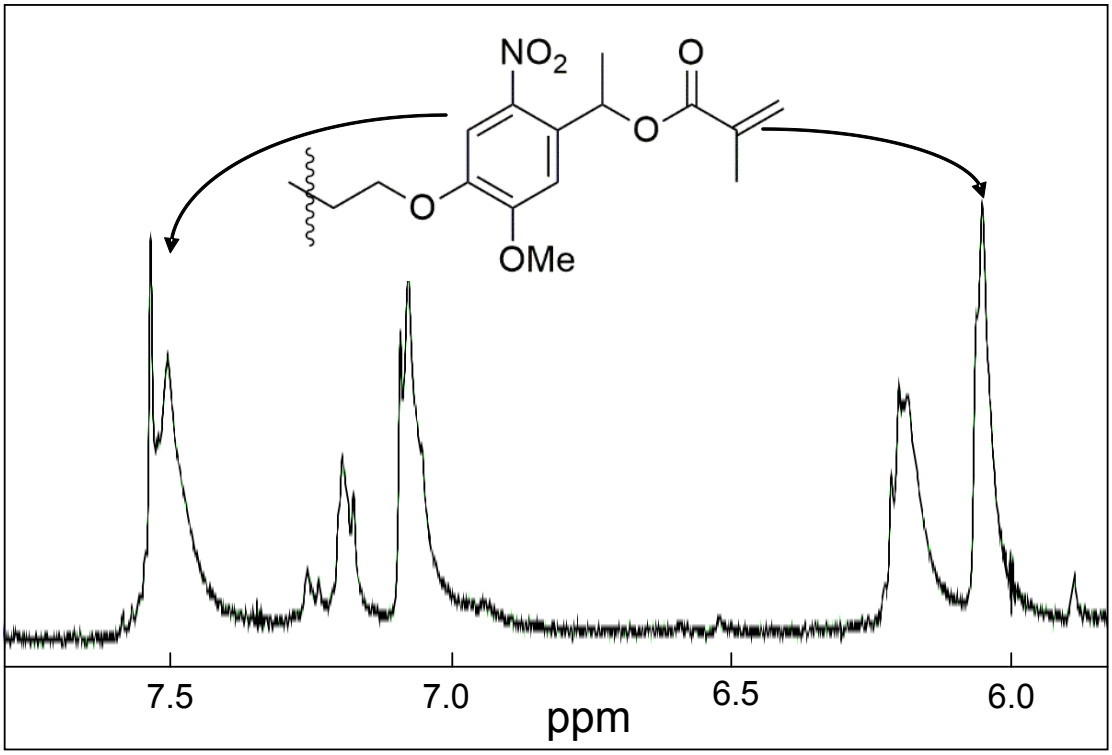

[kcal/mol]
Bond Potential Bead7-Bead8
Before
After
20
15
10
5
0
0
2
4
6
8
10
[Å]


[kcal/mol]
Bond Potential Bead2-Bead1
Before
After
20
15
10
5
0
0
2
4
6
8
10
[Å]

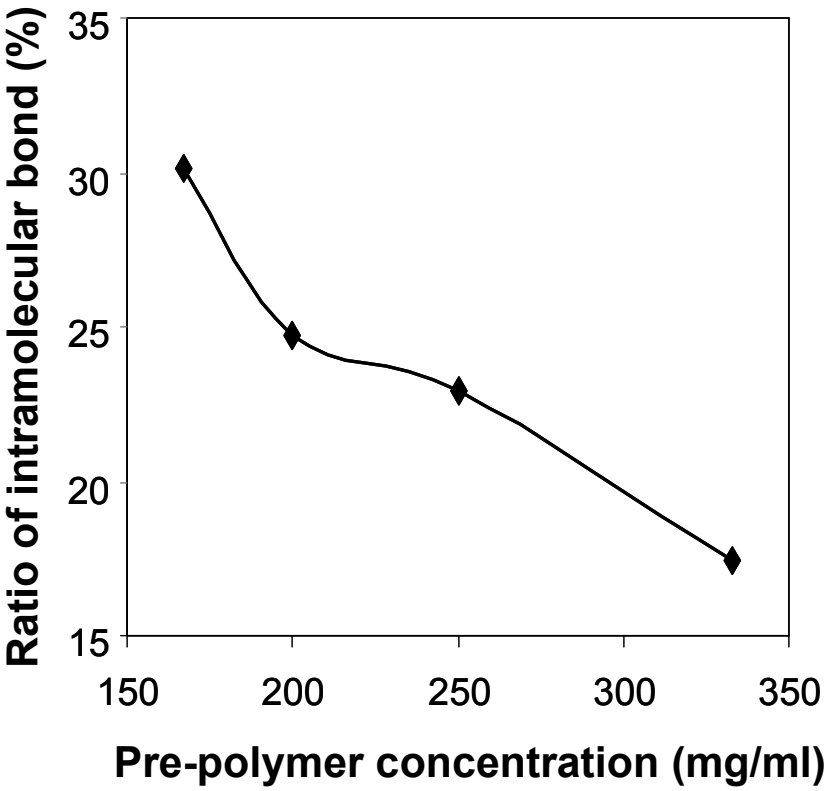

[kcal/mol]
Non bonded potential between Bead 1 – Bead 1
Before
After
1
0.75
0.5
0.25
0
-0.25
0
4
8
12
16
20
[Å]


[kcal/mol]
Non bonded potential between Bead 3(2) – Bead 7
Before
After
1
0.75
0.5
0.25
0
-0.25
0
4
8
12
16
20
[Å]

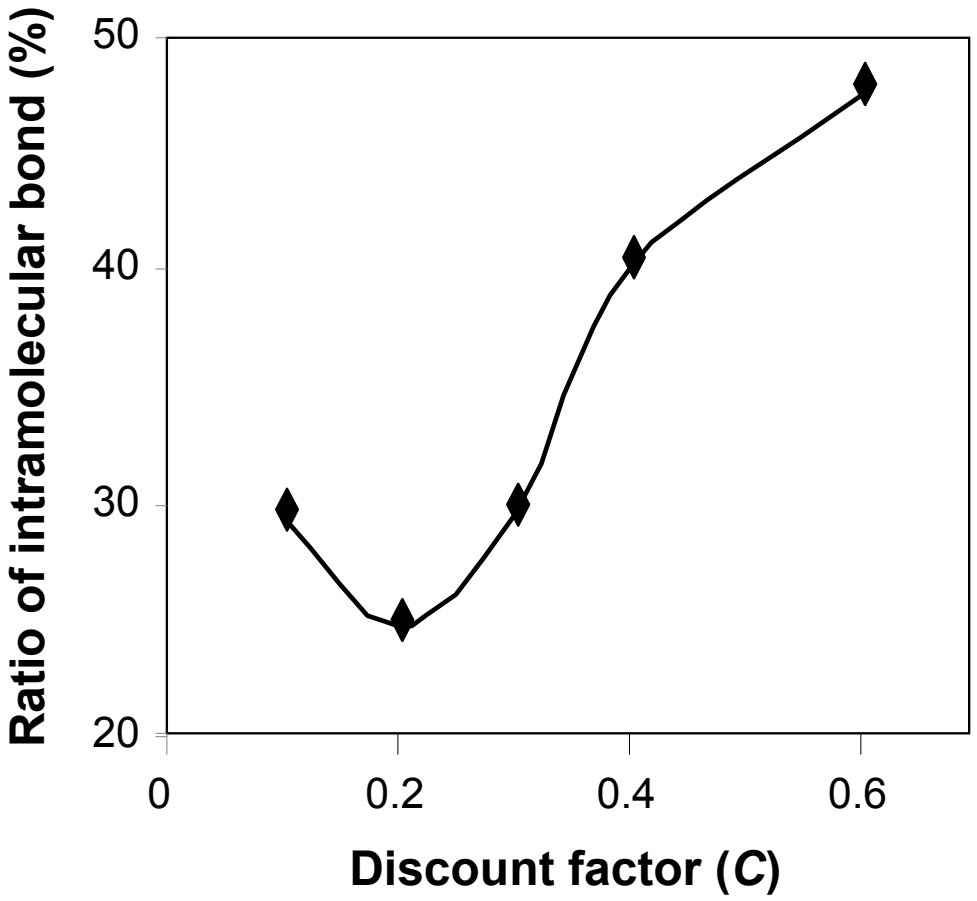
Supp. Fig. 1



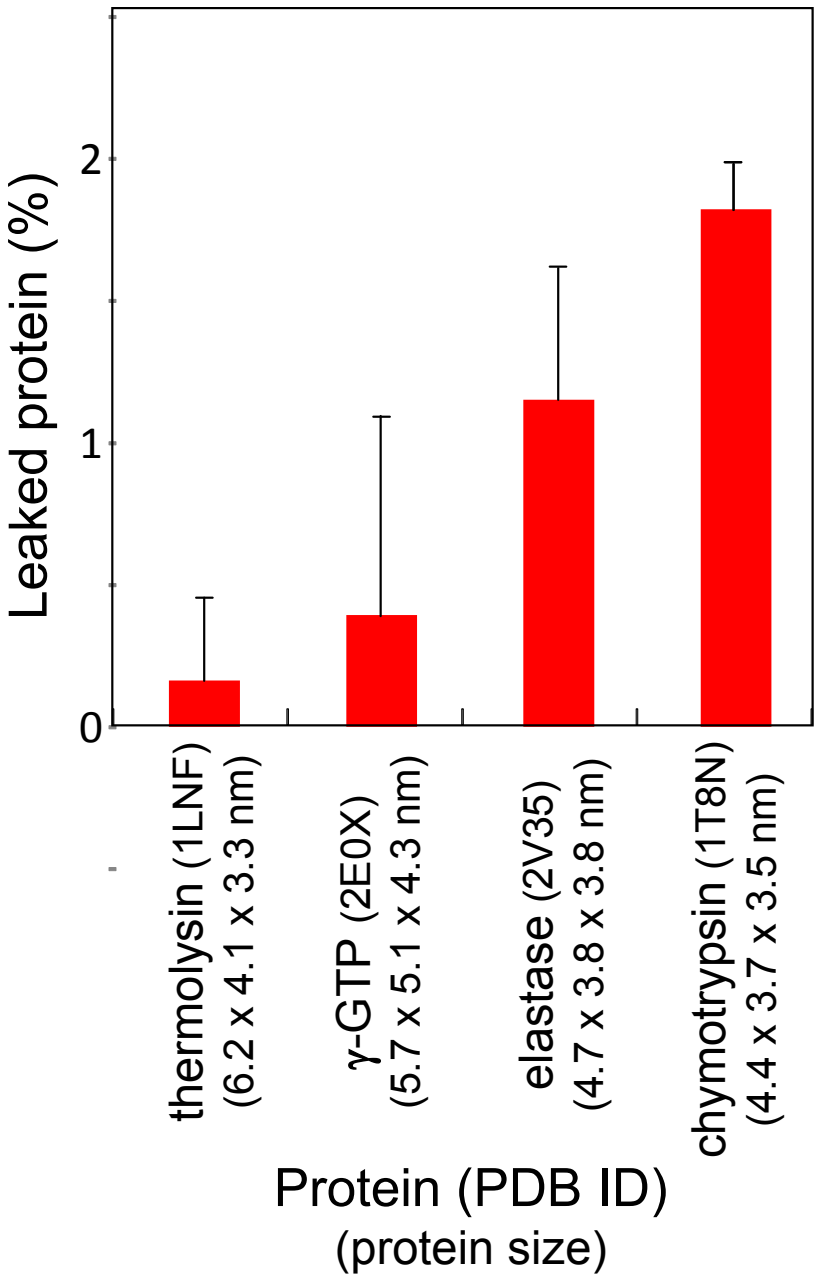
Supp. Fig. 2


Ratio of intramolecular bond (%)
35
30
25
20
15
150
200
250
300
350
Pre-polymer concentration (mg/ml)

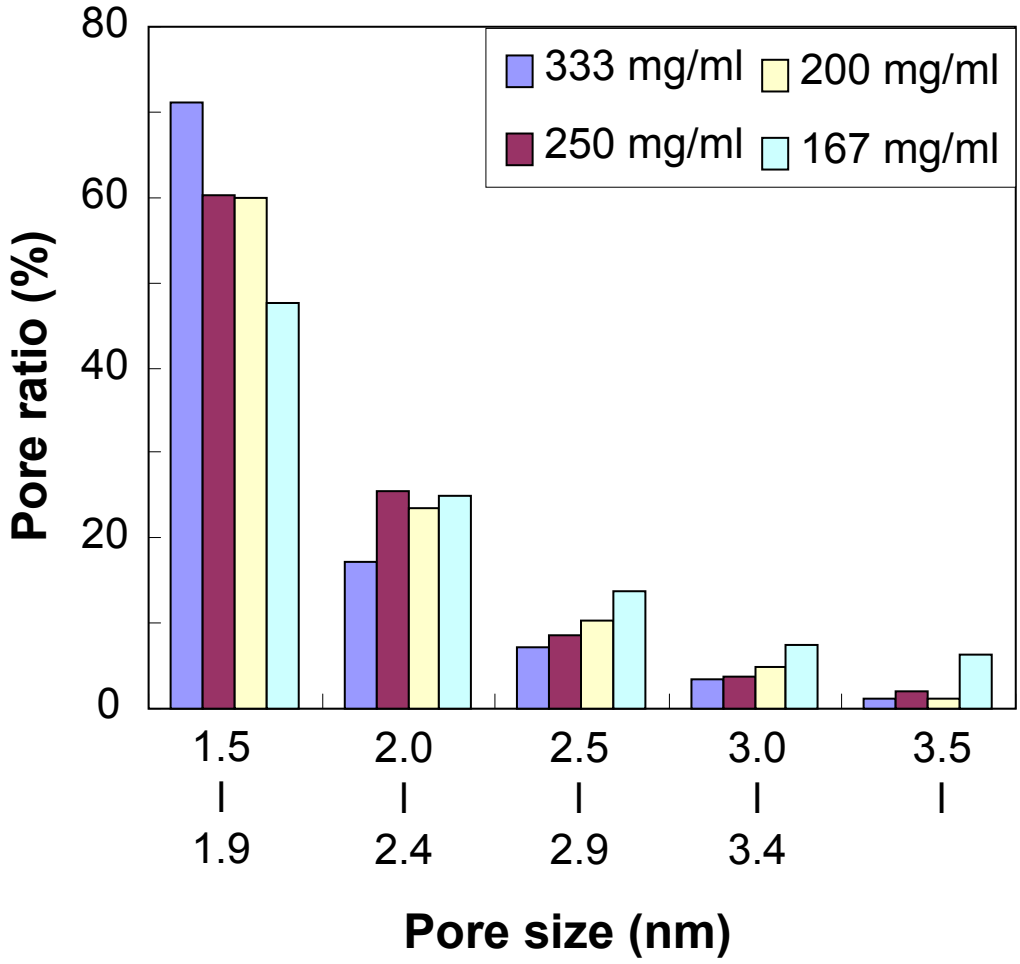
Supp. Fig. 3


Ratio of intramolecular bond (%)
50
40
30
20
0
0.2
0.4
0.6
Discount factor (C)

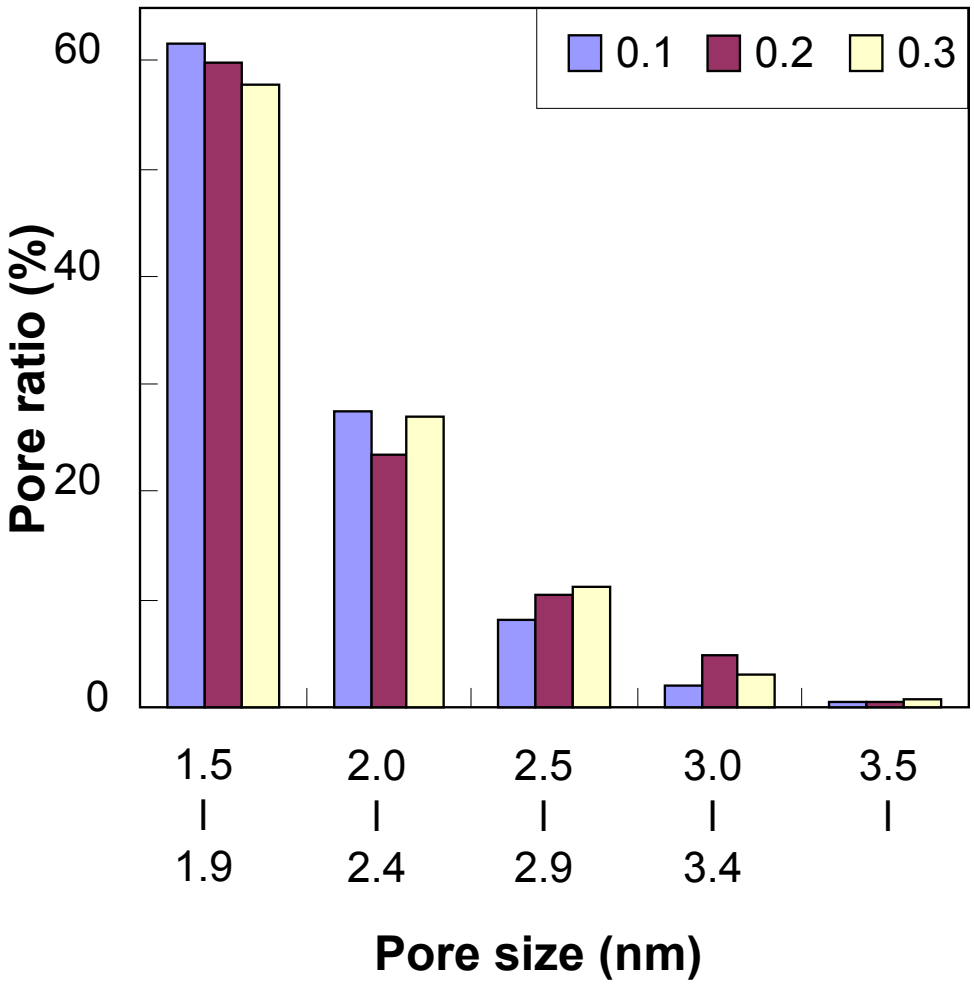
Supp. Fig. 4


Leaked protein (%)
0
1
2
thermolysin (1LNF)
(6.2 x 4.1 x 3.3 nm)
γ-GTP (2E0X)
(5.7 x 5.1 x 4.3 nm)
elastase (2V35)
(4.7 x 3.8 x 3.8 nm)
chymotrypsin (1T8N)
(4.4 x 3.7 x 3.5 nm)
Protein (PDB ID)
(protein size)

Supp. Fig. 5


80
60
40
20
0
Pore ratio (%)
333 mg/ml
200 mg/ml
250 mg/ml
167 mg/ml
1.5
|
1.9
2.0
|
2.4
2.5
|
2.9
3.0
|
3.4
3.5
|
Pore size (nm)

Supp. Fig. 6


0.1
0.2
0.3
60
40
20
0
Pore ratio (%)
1.5
|
1.9
2.0
|
2.4
2.5
|
2.9
3.0
|
3.4
3.5
|
Pore size (nm)

Supp. Fig. 7