

Assignments for 1H-1H TOCSY of commercial BPTI, acquired on 28/08/2008

Assignment	w1	w2
CYS5NH-NH	7.472	7.472
CYS5HA-NH	4.347	7.476
CYS5HB2-NH	2.859	7.477
CYS5HB3-NH	2.742	7.476
LEU6NH-NH	7.573	7.569
LEU6HA-NH	4.505	7.572
LEU6HB2-NH	1.842	7.571
GLU7NH-NH	7.524	7.524
GLU7HA-NH	4.58	7.522
GLU7HB2-NH	2.247	7.522
GLU7HB3-NH	2.167	7.522
TYR10NH-NH	7.804	7.801
TYR10HA-NH	4.93	7.808
TYR10HB2-NH	2.955	7.802
GLY12NH-NH	7.162	7.158
GLY12HA2-NH	3.896	7.16
GLY12HA3-NH	3.262	7.161
CYS14NH-NH	8.73	8.694
CYS14HA-NH	4.557	8.694
CYS14HB2-NH	3.463	8.694
CYS14HB3-NH	2.798	8.694
LYS15NH-NH	7.966	7.966
LYS15HA-NH	4.407	7.964
LYS15HB2-NH	2.09	7.964
LYS15HB3-NH	1.574	7.967
ALA16NH-NH	8.25	8.25
ALA16HA-NH	4.296	8.202
ALA16HB-NH	1.172	8.208
ARG17NH-NH	8.228	8.222
ARG17HA-NH	4.316	8.19
ARG17HB2-NH	1.594	8.193
ILE18NH-NH	8.17	8.119
ILE18HA-NH	4.195	8.117
ILE18HB-NH	1.866	8.118
ILE19NH-NH	8.69	8.69
ILE19HA-NH	4.306	8.69
ILE19HB-NH	1.947	8.69
ARG20NH-NH	8.401	8.401
ARG20HA-NH	4.697	8.392
ARG20HB2-NH	1.805	8.395
ARG20HB3-NH	0.811	8.395
TYR21NH-NH	9.185	9.184
TYR21HA-NH	5.68	9.185
TYR21HB2-NH	2.698	9.186
PHE22NH-NH	9.777	9.776
PHE22HA-NH	5.269	9.775
PHE22HB2-NH	2.907	9.777
PHE22HB3-NH	2.823	9.777
TYR23NH-NH	10.555	10.555
TYR23HA-NH	4.293	10.556
TYR23HB2-NH	3.462	10.555
TYR23HB3-NH	2.731	10.556

ASN24NH-NH	7.867	7.764
ASN24HA-NH	4.602	7.763
ASN24HB2-NH	2.857	7.762
ASN24HB3-NH	2.167	7.762
ALA25NH-NH	8.79	8.787
ALA25HA-NH	3.761	8.787
ALA25HB-NH	1.555	8.787
LYS26NH-NH	7.9	7.899
LYS26HA-NH	4.068	7.911
LYS26HB2-NH	1.885	7.913
ALA27NH-NH	6.86	6.821
ALA27HA-NH	4.289	6.816
ALA27HB-NH	1.182	6.817
GLY28NH-NH	8.14	8.14
GLY28HA2-NH	3.917	8.135
GLY28HA3-NH	3.612	8.135
LEU29NH-NH	6.86	6.824
LEU29HA-NH	4.748	6.819
LEU29HB2-NH	1.729	6.82
LEU29HB3-NH	1.427	6.82
CYS30NH-NH	8.44	8.415
CYS30HA-NH	5.606	8.408
CYS30HB2-NH	3.67	8.409
CYS30HB3-NH	2.662	8.407
GLN31NH-NH	8.768	8.77
GLN31HA-NH	4.824	8.764
GLN31HB2-NH	2.22	8.765
GLN31HB3-NH	1.728	8.765
THR32NH-NH	8.035	8.031
THR32HA-NH	5.289	8.034
THR32HB-NH	4.035	8.031
PHE33NH-NH	9.374	9.373
PHE33HA-NH	4.866	9.37
PHE33HB2-NH	3.084	9.368
PHE33HB3-NH	2.948	9.369
VAL34NH-NH	8.373	8.376
VAL34HA-NH	3.913	8.369
VAL34HB-NH	1.948	8.369
TYR35NH-NH	9.39	9.391
TYR35HA-NH	4.873	9.384
TYR35HB2-NH	2.664	9.388
TYR35HB3-NH	2.5	9.388
GLY36NH-NH	8.64	8.609
GLY36HA2-NH	4.317	8.608
GLY36HA3-NH	3.242	8.608
GLY37NH-NH	4.302	4.301
GLY37HA2-NH	4.219	4.315
GLY37HA3-NH	2.903	4.311
CYS38NH-NH	7.77	7.771
CYS38HA-NH	4.952	7.757
CYS38HB2-NH	3.959	7.757
CYS38HB3-NH	3.032	7.758
ALA40NH-NH	7.422	7.425
LYS41NH-NH	8.327	8.322
LYS41HA-NH	4.439	8.325
LYS41HB2-NH	2.252	8.326

LYS41HB3-NH	1.658	8.325
ARG42NH-NH	8.368	8.364
ARG42HA-NH	3.661	8.365
ARG42HB2-NH	1.03	8.365
ARG42HB3-NH	0.357	8.36
ASN43NH-NH	7.224	7.225
ASN43HA-NH	5.054	7.216
ASN43HB2-NH	3.33	7.216
ASN43HB3-NH	3.269	7.214
ASN44NH-NH	6.81	6.767
ASN44HA-NH	4.897	6.769
ASN44HB2-NH	2.775	6.769
ASN44HB3-NH	2.503	6.769
PHE45NH-NH	9.937	9.936
PHE45HA-NH	5.123	9.936
PHE45HB2-NH	3.402	9.94
PHE45HB3-NH	2.786	9.936
SER47NH-NH	7.5	7.447
SER47HA-NH	4.53	7.463
SER47HB2-NH	4.125	7.463
SER47HB3-NH	3.862	7.464
ALA48NH-NH	8.18	8.108
ALA48HA-NH	3.152	8.143
ALA48HB-NH	1.033	8.135
GLU49NH-NH	8.61	8.611
GLU49HA-NH	3.858	8.609
GLU49HB2-NH	1.999	8.61
GLU49HB3-NH	1.83	8.609
ASP50NH-NH	7.853	7.852
ASP50HA-NH	4.279	7.855
ASP50HB2-NH	2.87	7.854
ASP50HB3-NH	2.718	7.855
CYS51NH-NH	6.988	6.987
CYS51HA-NH	1.686	6.989
CYS51HB2-NH	3.172	6.989
CYS51HB3-NH	2.884	6.989
MET52NH-NH	8.593	8.591
MET52HA-NH	4.165	8.591
MET52HB2-NH	2.056	8.591
MET52HB3-NH	1.956	8.59
ARG53NH-NH	8.268	8.267
ARG53HA-NH	3.986	8.266
ARG53HB2-NH	1.918	8.266
ARG53HB3-NH	1.869	8.266
THR54NH-NH	7.394	7.393
THR54HA-NH	4.065	7.397
THR54HB-NH	4.005	7.397
CYS55NH-NH	8.235	8.232
CYS55HA-NH	4.617	8.233
CYS55HB2-NH	2.232	8.232
CYS55HB3-NH	1.998	8.232
GLY56NH-NH	8	8
GLY56HA2-NH	3.848	7.99
GLY57NH-NH	8.206	8.202
GLY57HA2-NH	3.948	8.189
GLY57HA3-NH	3.824	8.188

ALA58NH-NH	7.92	7.919
ALA58HA-NH	4.025	7.919
ALA58HB-NH	1.303	7.917

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate after 5 min in deuterium oxide NMR buffer, acq

Assignment	w1	w2	Fit Height
Gly12N-NH	110.686	8.595	42807365
Ala16N-NH	125.214	8.498	49478880
Arg17aN-NH	121.178	8.421	39283227
Arg17bN-NH	122.508	8.536	44959040
Ile18N-NH	119.719	8.198	41677813
Arg20N-NH	126.762	8.371	31605164
Phe22N-NH	118.684	9.729	33259416
Ala27N-NH	118.603	7.017	58609287
Gly28N-NH	107.651	8.220	53037358
Leu29N-NH	114.911	6.990	38983583
Tyr35N-NH	128.782	8.774	35604380
Gly36N-NH	108.847	8.360	61224232
Arg39N-NH	120.947	8.375	45590237
Ala40N-NH	123.773	8.216	69172133
Arg42N-NH	120.146	8.113	50940619
Asn43N-NH	119.800	8.664	38759249
Ser47N-NH	109.763	7.454	36424305
Ala48N-NH	125.237	8.298	36210743
Glu49N-NH	117.386	8.754	45570834
Cys51N-NH	118.498	7.119	37516989
Arg53N-NH	119.938	7.988	44361210
Thr54N-NH	111.828	7.560	47206483
Gly56N-NH	108.045	7.900	53021268
Gly57N-NH	108.448	8.124	84764843
Ala58aN-NH	128.867	7.929	152653308
Ala58bN-NH	129.080	8.026	89010589

uired on 23/09/2009

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate after 24 hours in deuterium oxide NMR buffer, :

Assignment	w1	w2	Fit Height
Leu6N-NH	113.792	7.704	51114877
Glu7N-NH	120.304	7.601	209626965
Ile18N-NH	125.898	8.267	157057231
Arg20N-NH	130.241	8.503	148753266
Tyr21N-NH	115.173	9.303	97660987
Phe22N-NH	119.955	9.868	134329541
Tyr23N-NH	124.911	10.706	99620193
Asn24N-NH	125.181	7.775	136686441
Leu29N-NH	114.870	6.940	383805085
Gln31N-NH	122.918	8.859	135229829
Phe33N-NH	119.082	9.459	194980301
Tyr35N-NH	129.698	9.579	130547598
Gly36N-NH	114.363	8.779	121161008
Lys41N-NH	121.173	8.451	45602999
Asn44N-NH	120.679	6.854	164439707
Phe45N-NH	122.735	10.062	104661441
Cys51N-NH	119.759	7.075	142325028
Met52N-NH	120.476	8.696	94362282
Arg53N-NH	122.017	8.332	104795107
Cys55N-NH	114.920	8.393	102359736

acquired on 24/09/2009 (dataset labelled 23/09/2009)

Assignments for HSQC of Wild Type BPTI after 5 min in deuterium oxide NMR buffer, acquired on 23/09/2

Assignment	w1	w2	Fit Height
Phe4N-NH	117.375	8.062	34899848
Cys5N-NH	121.643	7.627	171691468
Leu6N-NH	113.711	7.699	230037878
Glu7N-NH	120.339	7.600	194076114
Tyr10N-NH	123.513	7.962	85957316
Cys14N-NH	120.434	8.848	85783887
Ala16N-NH	123.616	8.290	198439887
Ile18N-NH	125.909	8.265	177156236
Ile19N-NH	128.501	8.934	31213582
Arg20N-NH	130.279	8.500	142836976
Tyr21N-NH	115.160	9.304	95545216
Phe22N-NH	119.963	9.867	111862168
Tyr23N-NH	124.864	10.708	94410851
Asn24N-NH	125.169	7.775	124827054
Ala27N-NH	118.743	6.911	25537680
Gly28N-NH	107.292	8.260	147413566
Leu29N-NH	114.841	6.940	317173324
Gln31N-NH	122.917	8.856	112212550
Thr32N-NH	108.474	8.197	59270440
Phe33N-NH	119.104	9.458	148004040
Val34N-NH	118.836	8.588	49934060
Tyr35N-NH	129.698	9.578	97036678
Gly36N-NH	114.374	8.779	107552542
Lys41N-NH	121.165	8.458	122672089
Asn43N-NH	116.316	7.281	24918519
Asn44N-NH	120.664	6.855	135091047
Phe45N-NH	122.701	10.060	76362408
Ala48N-NH	125.802	8.308	38500333
Cys51N-NH	119.781	7.075	161168567
Met52N-NH	120.560	8.697	160525665
Arg53N-NH	122.076	8.336	206200182
Thr54N-NH	113.397	7.493	171953032
Cys55N-NH	115.028	8.393	113856543
Gly56N-NH	108.074	8.218	126241994

Assignments for HSQC of Wild Type BPTI after 24 hours in deuterium oxide NMR buffer, acquired on 24/0

Assignment	w1	w2	Fit Height
Leu6N-NH	113.792	7.704	51114877
Glu7N-NH	120.304	7.601	209626965
Ile18N-NH	125.898	8.267	157057231
Arg20N-NH	130.241	8.503	148753266
Tyr21N-NH	115.173	9.303	97660987
Phe22N-NH	119.955	9.868	134329541
Tyr23N-NH	124.911	10.706	99620193
Asn24N-NH	125.181	7.775	136686441
Leu29N-NH	114.870	6.940	383805085
Gln31N-NH	122.918	8.859	135229829
Phe33N-NH	119.082	9.459	194980301
Tyr35N-NH	129.698	9.579	130547598
Gly36N-NH	114.363	8.779	121161008
Lys41N-NH	121.173	8.451	45602999
Asn44N-NH	120.679	6.854	164439707
Phe45N-NH	122.735	10.062	104661441
Cys51N-NH	119.759	7.075	142325028
Met52N-NH	120.476	8.696	94362282
Arg53N-NH	122.017	8.332	104795107
Cys55N-NH	114.920	8.393	102359736

09/2009 (dataset labelled 23/09/2009)

Assignments for 1H-1H TOCSY of (30-51, 5-14) BPTI Intermediate, acquired on 10/06/2009

Assignment	w1	w2
Gly12NH-NH	8.611	8.606
Gly12NH-HA	8.611	4.056
Gly12HA-NH	4.056	8.606
Lys15NH-NH	8.192	8.180
Lys15HA-NH	4.324	8.185
Lys15HB-NH	1.736	8.177
Ala16NH-NH	8.528	8.520
Ala16HB-NH	1.389	8.517
Arg17aNH-NH	8.454	8.449
Arg17aHA-NH	4.380	8.453
Ile18NH-NH	8.226	8.220
Ile18HA-NH	4.300	8.218
Ile18HB-NH	1.722	8.219
Ile19NH-NH	8.489	8.476
Ile19HA-NH	4.537	8.475
Ile19HB-NH	1.870	8.474
Ile19HG2-HA	0.729	4.509
Arg20NH-NH	8.391	8.387
Arg20HA-NH	4.799	8.387
Arg20HB-NH	1.086	8.387
Tyr21NH-NH	9.070	9.063
Tyr21HA-NH	5.686	9.068
Tyr21HB2-NH	2.766	9.069
Phe22NH-NH	9.728	9.719
Phe22HA-NH	5.437	9.718
Tyr23NH-NH	9.728	9.720
Tyr23HA-NH	4.519	9.718
Asn24NH-NH	8.104	8.097
Asn24HA-NH	4.634	8.100
Asn24HB2-NH	2.931	8.098
Ala25NH-NH	8.588	8.583
Lys26NH-NH	8.038	8.037
Lys26HA-NH	4.116	8.038
Ala27NH-NH	7.031	7.029
Ala27HA-NH	4.302	7.028
Ala27HB-NH	1.238	7.027
Gly28NH-NH	8.244	8.238
Gly28HA2-NH	3.959	8.245
Gly28HA3-NH	3.776	8.241
Leu29NH-NH	7.000	6.996
Leu29HA-NH	4.905	7.002
Leu29HB2-NH	1.714	7.006
Leu29HB3-NH	1.461	7.002
Cys30NH-NH	8.938	8.924
Cys30HA-NH	5.641	8.923
Cys30HB2-NH	3.730	8.927
Cys30HB3-NH	2.704	8.924
Gln31NH-NH	9.042	9.033
Gln31HA-NH	4.892	9.030
Gln31HB2-NH	2.000	9.033
Gln31HB3-NH	1.744	9.039
Thr32NH-NH	8.310	8.303

Thr32HA-NH	4.936	8.301
Phe33NH-NH	8.642	8.635
Phe33HA-NH	4.797	8.635
Phe33HB-NH	2.998	8.636
Val34HA-NH	4.071	8.510
Val34HB-NH	1.936	8.515
Tyr35NH-NH	8.788	8.780
Tyr35HA-NH	4.400	8.782
Tyr35HB-NH	2.795	8.775
Gly36NH-NH	8.383	8.379
Gly36HA-NH	3.997	8.373
Gly37NH-NH	8.320	8.313
Ser38NH-NH	8.371	8.367
Arg39NH-NH	8.367	8.361
Arg39HA-NH	4.442	8.361
Ala40NH-NH	8.232	8.229
Ala40HA-NH	4.265	8.232
Ala40HB-NH	1.369	8.227
Lys41NH-NH	8.922	8.921
Lys41HA-NH	4.301	8.921
Arg42NH-NH	8.117	8.113
Arg42HA-NH	4.321	8.112
Asn43NH-NH	8.665	8.660
Asn43HA-NH	4.691	8.660
Asn44HA-NH	5.396	7.960
Phe45NH-NH	9.316	9.320
Phe45HA-NH	5.121	9.320
Lys46NH-NH	9.958	9.948
Lys46HA-NH	4.471	9.955
Ser47NH-NH	7.515	7.513
Ser47HA-NH	4.559	7.512
Ala48NH-NH	8.336	8.330
Glu49NH-NH	8.763	8.756
Glu49HA-NH	3.871	8.750
Asp50NH-NH	7.940	7.923
Asp50HA-NH	4.291	7.923
Cys51NH-NH	7.121	7.117
Met52NH-NH	8.668	8.668
Met52HA-NH	4.125	8.674
Arg53NH-NH	7.989	7.993
Arg53HA-NH	4.047	7.991
Thr54NH-NH	7.576	7.570
Thr54HA-NH	4.193	7.573
Thr54HB-NH	4.058	7.578
Ser55NH-NH	7.773	7.767
Ser55HA-NH	4.142	7.765
Ser55HB-NH	3.126	7.768
Ser55HB-NH	3.238	7.769
Gly56NH-NH	7.924	7.921
Gly56HA-NH	3.888	7.914
Gly57NH-NH	8.140	8.136
Gly57HA-NH	3.966	8.133
Ala58aNH-NH	7.956	7.950
Ala58aHA-NH	4.194	7.949
Ala58aHB-NH	1.364	7.949
Ala58bNH-NH	8.053	8.049

Ala58bHA-NH	4.182	8.048
Ala58bHB-NH	1.380	8.048

Assignments for 1H-1H NOESY of (30-51, 5-14) BPTI Intermediate, acquired on 10/06/2009

Assignment	w1	w2
Gly12NH-NH	8.607	8.604
Gly12HA-NH	4.058	8.603
Lys15NH-NH	8.185	8.182
Lys15HA-Ala16NH	4.316	8.535
Ala16NH-NH	8.524	8.523
Ala16HB-NH	1.390	8.520
Arg17aNH-NH	8.448	8.449
Arg17aHA-NH	4.396	8.449
Arg17aHB2-NH	1.801	8.542
Arg17bNH-NH	8.544	8.541
Arg17bHG2-NH	1.648	8.544
Arg17bHG3-NH	1.570	8.545
Ile18NH-Arg17aHB2	8.238	1.586
Ile18NH-Arg17aHB3	8.241	1.475
Ile18NH-Arg17bNH	8.230	8.544
Ile18NH-NH	8.224	8.220
Ile18NH-HA	8.235	4.199
Ile18NH-Ile19HA	8.231	4.307
Ile18NH-Ile19HB	8.228	1.856
Ile18HA-Arg17bNH	4.248	8.556
Ile18HA-NH	4.314	8.227
Ile18HA-Ile19NH	4.226	8.473
Ile18HB-NH	1.719	8.215
Ile18HB-HA	1.864	4.197
Ile19NH-NH	8.479	8.477
Ile19HA-Arg20NH	4.509	8.386
Ile19HB-Ile18NH	1.856	8.229
Ile19HB-NH	1.871	8.472
Ile19HG12-NH	1.454	8.473
Ile19HG2-NH	0.731	8.475
Ile19HG2-HA	0.734	4.508
Ile19HG2-Arg20NH	0.730	8.382
Arg20NH-NH	8.382	8.383
Arg20NH-Thr32HG	8.382	0.732
Arg20HA-NH	4.803	8.372
Arg20HA-Tyr21NH	4.802	9.065
Arg20HA-Tyr21HD	4.804	6.721
Arg20HA-Tyr21HE	4.808	6.801
Arg20HB-NH	1.089	8.383
Tyr21NH-NH	9.063	9.062
Tyr21NH-HB2	9.066	2.752
Tyr21NH-HD	9.063	6.716
Tyr21NH-Phe22NH	9.037	9.720
Tyr21HA-HD	5.676	6.714
Tyr21HA-HE	4.520	6.568
Tyr21HA-HE	5.670	6.800
Tyr21HA-Phe22NH	5.677	9.720
Tyr21HA-Phe22HE	5.674	7.182
Tyr21HB2-NH	2.769	9.062
Tyr21HB2-HD	2.762	6.715
Tyr21HB2-HE	2.760	6.802
Tyr21HB2-Phe22NH	2.759	9.717

Tyr21HB3-NH	2.686	9.063
Tyr21HB3-HD	2.696	6.715
Tyr21HB3-HE	2.693	6.802
Tyr21HB3-Phe22NH	2.693	9.721
Tyr21HD-NH	6.711	9.061
Phe22NH-NH	9.721	9.718
Phe22NH-HB2	9.714	3.203
Phe22NH-HB3	9.721	3.023
Phe22NH-HD	9.719	7.178
Phe22NH-Gln31NH	9.721	9.034
Phe22HA-NH	5.436	9.718
Phe22HA-HB2	5.431	3.203
Phe22HA-HB3	5.431	3.034
Phe22HA-HE	5.430	7.177
Phe22HB2-NH	3.203	9.718
Phe22HB2-HE	3.201	7.182
Phe22HB3-NH	3.022	9.719
Phe22HB3-HE	3.022	7.182
Phe22HD-NH	7.179	9.719
Phe22HE-NH	7.299	9.715
Tyr23NH-NH	9.721	9.719
Tyr23NH-HD	9.713	7.094
Tyr23NH-Phe45HD	9.713	7.295
Tyr23HA-NH	4.526	9.719
Tyr23HA-HB	4.522	3.017
Tyr23HA-HD	4.524	7.095
Tyr23HA-Asn24NH	4.530	8.093
Tyr23HA-Gln31NH	4.525	9.033
Tyr23HB-HE	3.018	6.570
Tyr23HD-NH	7.099	9.720
Tyr23HE-HD	6.572	7.099
Asn24NH-NH	8.097	8.094
Asn24HA-NH	4.637	8.099
Asn24HA-Ala25NH	4.636	8.584
Asn24HB2-NH	2.929	8.098
Asn24HB3-NH	2.283	8.097
Ala25NH-NH	8.585	8.584
Ala25NH-HB	8.585	1.583
Ala25NH-Lys26NH	8.579	8.033
Ala25HA-HB	3.707	1.585
Ala25HB-NH	1.579	8.584
Lys26NH-Ala25NH	8.033	8.582
Lys26NH-NH	8.035	8.031
Lys26NH-Ala27NH	8.034	7.026
Lys26HA-NH	4.114	8.032
Lys26HA-Ala27NH	4.105	7.024
Lys26HB-NH	1.940	8.031
Lys26HB-Ala27NH	1.937	7.028
Lys26HG-NH	1.577	8.035
Ala27NH-Lys26NH	7.022	8.036
Ala27NH-NH	7.025	7.025
Ala27NH-Gly28NH	7.015	8.247
Ala27HA-NH	4.305	7.024
Ala27HA-HB	4.301	1.241
Ala27HB-NH	1.243	7.025
Ala27HB-Gly28NH	1.237	8.246

Gly28NH-Ala27NH	8.246	7.014
Gly28NH-Ala27HB	8.247	1.241
Gly28NH-NH	8.239	8.237
Gly28HA2-NH	3.960	8.246
Gly28HA2-Leu29NH	3.961	7.001
Gly28HA3-NH	3.765	8.247
Gly28HA3-Leu29NH	3.766	7.002
Leu29NH-NH	7.003	6.999
Leu29HA-Phe22HD	4.898	7.184
Leu29HA-NH	4.909	7.001
Leu29HA-Cys30NH	4.910	8.923
Leu29HB2-NH	1.725	7.000
Leu29HB2-Cys30NH	1.726	8.921
Leu29HB3-NH	1.469	7.002
Leu29HB3-Cys30NH	1.468	8.924
Cys30NH-NH	8.925	8.926
Cys30NH-HB3	8.922	2.704
Cys30NH-Thr32HG	8.905	0.734
Cys30HA-Tyr23HD	5.630	7.096
Cys30HA-Asn24NH	5.630	8.095
Cys30HA-NH	5.634	8.922
Cys30HA-Gln31NH	5.632	9.028
Cys30HB2-NH	3.724	8.923
Cys30HB3-NH	2.703	8.926
Cys30HB3-Gln31NH	2.696	9.036
Gln31NH-NH	9.037	9.034
Gln31HA-NH	4.900	9.026
Gln31HA-Thr32NH	4.897	8.301
Gln31HB2-NH	2.004	9.026
Gln31HB2-Thr32NH	2.012	8.304
Gln31HB3-NH	1.741	9.033
Gln31HB3-Thr32NH	1.743	8.300
Gln31HB3-Thr32HB	1.739	4.047
Gln31HG-NH	2.095	9.028
Gln31HG-Thr32NH	2.092	8.299
Thr32NH-NH	8.304	8.301
Thr32NH-HG	8.301	0.736
Thr32HA-HB	4.941	4.047
Thr32HA-HG	4.939	0.735
Thr32HG-Tyr21HD	0.732	6.719
Thr32HG-Tyr21HE	0.735	6.802
Thr32HG-NH	0.733	8.301
Phe33NH-NH	8.634	8.632
Phe33HA-HB2	4.896	3.195
Phe33HA-HB3	4.896	3.024
Phe33HA-Val34NH	4.895	8.508
Phe33HB-NH	2.991	8.624
Val34NH-Phe33HB3	8.506	3.027
Val34NH-HG2	8.507	0.876
Val34HA-NH	4.072	8.504
Val34HA-HG1	4.076	0.830
Val34HA-HG2	4.077	0.874
Val34HA-Tyr35NH	4.075	8.775
Val34HB-NH	1.951	8.511
Val34HG-NH	0.874	8.507
Tyr35NH-Val34NH	8.754	8.512

Tyr35NH-NH	8.778	8.779
Tyr35NH-HB3	8.775	2.504
Tyr35HA-NH	4.393	8.782
Tyr35HB-NH	2.811	8.776
Gly36NH-NH	8.378	8.376
Gly36HA-NH	3.981	8.361
Gly36HA2-Gly37HA2	3.980	3.842
Gly37NH-NH	8.317	8.313
Ser38NH-NH	8.369	8.367
Ser38HA-HB2	4.425	3.966
Ser38HA-HB3	4.424	3.896
Arg39NH-Ser38HA	8.352	4.423
Arg39NH-NH	8.352	8.348
Arg39HA-NH	4.411	8.346
Ala40NH-Arg39HB	8.227	1.787
Ala40NH-NH	8.231	8.229
Ala40NH-HB	8.226	1.358
Ala40HA-NH	4.262	8.225
Ala40HB-NH	1.364	8.230
Lys41NH-NH	8.925	8.919
Lys41HA-NH	4.301	8.915
Arg42NH-NH	8.113	8.111
Arg42NH-HA	8.111	4.317
Arg42HA-NH	4.317	8.112
Arg42HA-Asn43NH	4.321	8.659
Arg42HB-NH	1.855	8.112
Arg42HB-HA	1.854	4.313
Arg42HG-NH	1.607	8.110
Arg42HG-HA	1.610	4.317
Asn43NH-Arg42NH	8.648	8.113
Asn43NH-Arg42HA	8.659	4.318
Asn43NH-NH	8.661	8.659
Asn43HA-NH	4.690	8.658
Asn43HA-HB	4.690	2.799
Asn43HA-Asn44NH	4.691	7.960
Asn43HB-NH	2.808	8.661
Asn44HA-Phe45NH	5.390	9.312
Phe45NH-Tyr23HB3	9.315	2.735
Phe45NH-NH	9.318	9.314
Phe45NH-HB2	9.317	2.770
Phe45NH-HD	9.314	7.295
Phe45HA-NH	5.103	9.313
Phe45HA-Lys46NH	5.101	9.948
Phe45HB2-NH	2.763	9.318
Phe45HD-NH	7.293	9.315
Lys46NH-NH	9.949	9.947
Lys46NH-Ser47NH	9.956	7.514
Lys46HA-NH	4.476	9.944
Lys46HB-NH	2.069	9.952
Lys46HG-NH	1.579	9.950
Ser47NH-Lys46NH	7.503	9.950
Ser47NH-NH	7.510	7.510
Ser47HA-Tyr21HD	4.558	6.717
Ser47HA-Tyr21HE	4.559	6.802
Ser47HA-NH	4.559	7.508
Ser47HA-HB2	4.551	4.136

Ser47HA-HB3	4.557	3.874
Ser47HA-Ala48NH	4.557	8.328
Ser47HA-Glu49NH	4.553	8.745
Ser47HB2-Ala48NH	4.133	8.330
Ala48NH-Ser47HB2	8.329	4.134
Ala48NH-NH	8.333	8.330
Ala48NH-HA	8.329	3.109
Ala48NH-HB	8.328	1.110
Ala48NH-Glu49NH	8.328	8.747
Ala48HA-Tyr21HD	3.110	6.715
Ala48HA-Tyr21HE	3.108	6.802
Ala48HA-NH	3.107	8.328
Ala48HB-Tyr21HD	1.105	6.715
Ala48HB-Tyr21HE	1.107	6.801
Ala48HB-NH	1.108	8.328
Ala48HB-Glu49NH	1.107	8.748
Glu49NH-Ala48NH	8.748	8.330
Glu49NH-Ala48HB	8.746	1.110
Glu49NH-NH	8.754	8.751
Glu49NH-HB2	8.745	2.016
Glu49NH-HB3	8.742	1.852
Glu49NH-Asp50NH	8.748	7.922
Glu49HA-NH	3.869	8.748
Glu49HA-Met52NH	3.866	8.672
Glu49HB2-NH	2.023	8.748
Glu49HB3-NH	1.853	8.747
Glu49HB3-HA	1.850	3.867
Asp50NH-Glu49NH	7.921	8.747
Asp50NH-NH	7.928	7.923
Asp50NH-Cys51NH	4.276	7.117
Asp50HA-NH	4.293	7.922
Asp50HA-HB3	4.292	2.721
Asp50HB-NH	2.719	7.922
Asp50HB-Cys51NH	2.719	7.113
Cys51NH-Asp50NH	7.112	7.921
Cys51NH-NH	7.112	7.112
Cys51NH-Met52NH	7.113	8.670
Cys51HB2-NH	2.814	7.114
Cys51HB3-NH	2.500	7.114
Met52NH-Cys51HB2	8.671	3.169
Met52NH-Cys51HB3	8.664	2.815
Met52NH-NH	8.668	8.668
Met52NH-HB2	8.671	2.051
Met52NH-HG	8.672	2.682
Met52NH-Arg53NH	8.668	7.991
Met52HA-NH	4.124	8.669
Met52HA-Arg53NH	4.122	7.992
Met52HB-NH	2.053	8.669
Met52HG-NH	2.679	8.669
Arg53NH-Met52NH	7.989	8.669
Arg53NH-NH	7.989	7.991
Arg53NH-Thr54NH	7.988	7.573
Arg53HA-NH	4.048	7.991
Arg53HB-NH	1.921	7.992
Arg53HG-NH	1.621	7.993
Arg53HG-HA	1.625	4.048

Thr54NH-Arg53NH	7.568	7.991
Thr54NH-NH	7.571	7.569
Thr54NH-Ser55NH	7.572	7.768
Thr54HA-NH	4.192	7.570
Thr54HB-NH	4.052	7.571
Thr54HB-Ser55NH	4.056	7.769
Thr54HG-NH	1.378	7.575
Ser55NH-Thr54NH	7.764	7.572
Ser55NH-NH	7.767	7.765
Ser55NH-Gly56NH	7.771	7.920
Ser55HA-Glu49NH	4.135	8.749
Ser55HA-NH	4.138	7.767
Ser55HA-HB2	4.142	3.240
Ser55HA-HB3	4.139	3.133
Ser55HA-Gly56NH	4.135	7.919
Ser55HB-NH	3.126	7.767
Ser55HB-NH	3.243	7.770
Gly56NH-NH	7.920	7.917
Gly56NH-Gly57NH	7.926	8.136
Gly56HA-NH	3.886	7.919
Gly57NH-Gly56NH	8.130	7.919
Gly57NH-NH	8.133	8.133
Gly57HA-NH	3.944	8.134
Ala58aNH-NH	7.950	7.948
Ala58aHA-NH	4.197	7.949
Ala58aHB-NH	1.367	7.947
Ala58bNH-NH	8.047	8.047
Ala58bHA-NH	4.191	8.046
Ala58bHB-NH	1.381	8.046

Assignments for 1H-15N-1H NOESY (HSQC-NOESY) of (30-51, 5-14) BPTI Intermediate, acquired on

Assignment	w1	w2	w3
Lys15H-N-H	8.171	120.102	8.17
Ala16H-N-H	8.526	125.143	8.518
Ala16HA-Arg17aN-H	4.274	121.05	8.457
Arg17aH-N-H	8.464	121.196	8.457
Ile18H-N-H	8.222	119.953	8.222
Ile18HA-Ile19N-H	4.188	126.577	8.467
Ile19H-N-H	8.484	126.693	8.47
Ile19HA-Arg20N-H	4.499	126.466	8.379
Arg20H-N-H	8.368	126.578	8.377
Tyr21HA-Phe22N-H	5.68	119.257	9.717
Phe22H-N-H	9.729	119.445	9.716
Asn24HA-Ala25N-H	4.621	126.951	8.583
Ala25H-N-H	8.574	126.987	8.579
Ala27H-Gly28N-H	7.004	107.861	8.237
Gly28H-N-H	8.236	107.825	8.237
Gly28HA2-N-H	3.956	107.775	8.239
Gly28HA3-N-H	3.733	107.892	8.236
Leu29HA-Cys30N-H	4.891	119.158	8.923
Cys30H-N-H	8.927	119.236	8.924
Phe33H-N-H	8.65	119.045	8.651
Val34H-N-H	8.506	120.746	8.507
Val34HA-Tyr35N-H	4.054	128.939	8.764
Tyr35H-N-H	8.767	128.987	8.77
Arg39H-N-H	8.368	120.98	8.371
Arg42H-N-H	8.117	119.934	8.116
Asn43H-N-H	8.672	119.915	8.665
Asn43HA-Arg42N-H	4.309	120.193	8.665
Phe45H-N-H	9.347	117.068	9.311
Ser47HA-Ala48N-H	4.547	125.26	8.325
Ala48H-N-H	8.327	125.225	8.325
Asp50H-N-H	7.92	119.933	7.917
Met52H-N-H	8.656	121.361	8.663
Arg53H-N-H	7.976	120.004	7.977
Arg53HA-N-H	4.057	119.959	7.976
Arg53HB-N-H	1.907	120.285	7.977
Arg53HB-Thr54N-H	1.843	112.075	7.563
Thr54H-N-H	7.555	111.998	7.563
Thr54H-Ser55N-H	7.588	115.638	7.762
Ser55H-N-H	7.76	115.604	7.763
Ser55H-Gly56N-H	7.769	108.562	7.92
Gly56H-N-H	7.916	108.25	7.918
Gly56HA-N-H	3.893	108.561	7.919
Gly57H-N-H	8.127	108.764	8.128
Gly57HA2-N-H	3.919	108.786	8.128
Ala58aH-N-H	7.944	128.803	7.943
Ala58aHB-N-H	1.39	128.614	7.944
Ala58bH-N-H	8.039	129.001	8.041

06/02/2009

Assignments for 1H-15N-1H TOCSY (HSQC-TOCSY) of (30-51, 5-14) BPTI Intermediate, acquired

Assignment	w1	w2	w3
Gly12NH-N-NH	8.583	110.807	8.596
Gly12HA-N-NH	4.036	110.747	8.596
Lys15NH-N-NH	8.166	120.003	8.167
Lys15HA-N-NH	4.308	120.007	8.169
Lys15HB-N-NH	1.708	120.001	8.168
Ala16NH-N-NH	8.502	125.264	8.517
Ala16HA-N-NH	4.269	125.353	8.518
Ala16HB-N-NH	1.381	125.234	8.517
Arg17aNH-N-NH	8.447	121.033	8.454
Arg17aHA-N-NH	4.383	121.025	8.454
Arg17aHB-N-NH	1.766	121.135	8.454
Arg17bNH-N-NH	8.537	122.624	8.548
Arg17bHA-N-NH	4.288	122.695	8.546
Arg17bHB-N-NH	1.794	122.698	8.547
Arg17bHG-N-NH	1.612	122.687	8.548
Ile18NH-N-NH	8.214	119.903	8.218
Ile18HA-N-NH	4.299	119.942	8.220
Ile18HB-N-NH	1.706	119.856	8.218
Ile18HG12-N-NH	1.511	120.039	8.220
Ile18HG13-N-NH	1.226	119.758	8.218
Ile19NH-N-NH	8.461	126.782	8.468
Ile19HA-N-NH	4.496	126.819	8.472
Ile19HB-N-NH	1.829	126.703	8.467
Ile19HG12-N-NH	1.479	126.920	8.471
Ile19HG2-N-NH	0.725	126.905	8.468
Arg20NH-N-NH	8.381	126.622	8.379
Arg20HA-N-NH	4.794	126.630	8.381
Arg20HB-N-NH	1.077	126.645	8.376
Tyr21NH-N-NH	9.068	115.466	9.053
Phe22NH-N-NH	9.700	119.466	9.707
Phe22HA-N-NH	5.407	119.247	9.710
Tyr23NH-N-NH	9.686	123.238	9.705
Tyr23HA-N-NH	4.494	123.017	9.709
Tyr23HB-N-NH	3.004	122.984	9.705
Asn24NH-N-NH	8.081	127.697	8.094
Asn24HA-N-NH	4.617	127.798	8.096
Asn24HB2-N-NH	2.925	127.708	8.092
Asn24HB3-N-NH	2.275	127.805	8.087
Ala25NH-N-NH	8.558	127.041	8.578
Ala25HB-N-NH	1.566	126.905	8.578
Lys26NH-N-NH	8.009	117.495	8.025
Lys26HA-N-NH	4.098	117.490	8.025
Lys26HB-N-NH	1.925	117.495	8.026
Lys26HG-N-NH	1.508	117.476	8.024
Ala27NH-N-NH	7.003	118.615	7.016
Ala27HA-N-NH	4.288	118.628	7.017
Ala27HB-N-NH	1.239	118.621	7.018
Gly28NH-N-NH	8.228	107.703	8.235
Gly28HA2-N-NH	3.955	107.620	8.235
Gly28HA3-N-NH	3.761	107.710	8.233
Leu29NH-N-NH	6.980	114.999	6.995
Leu29HA-N-NH	4.887	115.023	6.995

Leu29HB2-N-NH	1.718	115.005	6.996
Leu29HB3-N-NH	1.462	115.073	6.994
Cys30NH-N-NH	8.916	119.181	8.923
Cys30HA-N-NH	5.624	119.173	8.920
Cys30HB-N-NH	2.698	119.043	8.917
Gln31NH-N-NH	9.013	122.605	9.020
Gln31HA-N-NH	4.863	122.582	9.023
Gln31HB2-N-NH	1.976	122.718	9.020
Gln31HB3-N-NH	1.723	122.701	9.028
Gln31HG-N-NH	2.239	122.765	9.024
Thr32NH-N-NH	8.284	110.298	8.293
Thr32HA-N-NH	4.934	110.427	8.295
Phe33NH-N-NH	8.645	118.727	8.645
Phe33HA-N-NH	4.768	118.751	8.644
Phe33HB-N-NH	2.991	118.855	8.647
Val34NH-N-NH	8.498	120.618	8.505
Val34HA-N-NH	4.059	120.662	8.508
Val34HB-N-NH	1.937	120.680	8.507
Val34HG-N-NH	0.848	120.707	8.507
Tyr35NH-N-NH	8.770	129.239	8.765
Tyr35HA-N-NH	4.370	129.241	8.760
Tyr35HB-N-NH	2.857	129.241	8.768
Tyr35HD-N-NH	6.940	129.241	8.765
Gly36NH-N-NH	8.370	109.002	8.371
Gly36HA-N-NH	3.992	108.638	8.371
Gly37NH-N-NH	8.314	114.690	8.313
Gly37HA-N-NH	3.878	114.783	8.318
Ser38NH-N-NH	8.382	115.513	8.366
Ser38HA-N-NH	4.409	115.694	8.368
Ser38HB2-N-NH	3.923	115.694	8.367
Arg39NH-N-NH	8.364	121.007	8.368
Arg39HA-N-NH	4.448	121.072	8.367
Arg39HB-N-NH	1.782	121.050	8.370
Ala40NH-N-NH	8.209	123.857	8.218
Ala40HA-N-NH	4.242	123.876	8.219
Ala40HB-N-NH	1.358	123.870	8.217
Lys41NH-N-NH	8.916	124.060	8.921
Lys41HA-N-NH	4.288	123.862	8.921
Lys41HB-N-NH	1.771	124.030	8.921
Arg42NH-N-NH	8.105	120.029	8.116
Arg42HA-N-NH	4.300	120.211	8.117
Arg42HB-N-NH	1.832	120.219	8.119
Arg42HG-N-NH	1.593	120.157	8.116
Arg42HG-N-NH	1.596	120.313	8.114
Asn43NH-N-NH	8.656	119.852	8.662
Asn43HA-N-NH	4.667	119.887	8.661
Asn43HB-N-NH	2.777	119.744	8.662
Asn44NH-N-NH	7.962	117.780	7.961
Asn44HA-N-NH	5.366	117.652	7.963
Lys46NH-N-NH	9.971	120.181	9.950
Lys46HA-N-NH	4.463	120.281	9.950
Ser47NH-N-NH	7.482	109.355	7.503
Ser47HA-N-NH	4.535	109.471	7.503
Ala48NH-N-NH	8.318	125.304	8.323
Ala48HA-N-NH	3.122	125.270	8.323
Ala48HB-N-NH	1.098	125.357	8.324

Glu49NH-N-NH	8.739	117.564	8.747
Glu49HA-N-NH	3.854	117.574	8.749
Asp50NH-N-NH	7.911	119.844	7.917
Asp50HA-N-NH	4.276	119.821	7.916
Asp50HB-N-NH	2.712	119.713	7.917
Cys51NH-N-NH	7.085	118.545	7.105
Met52NH-N-NH	8.648	121.278	8.661
Met52HA-N-NH	4.109	121.291	8.662
Met52HB-N-NH	2.038	121.281	8.661
Arg53NH-N-NH	7.967	119.975	7.979
Arg53HA-N-NH	4.033	120.014	7.978
Arg53HB-N-NH	1.881	120.093	7.978
Arg53HE-N-NH	7.795	120.093	7.978
Arg53HG-N-NH	1.604	119.961	7.972
Thr54NH-N-NH	7.552	111.731	7.562
Thr54HA-N-NH	4.178	111.828	7.562
Thr54HB-N-NH	4.029	111.828	7.560
Thr54HG-N-NH	1.362	111.731	7.562
Ser55NH-N-NH	7.751	115.458	7.760
Ser55HA-N-NH	4.122	115.472	7.761
Ser55HB-N-NH	3.184	115.446	7.762
Gly56NH-N-NH	7.915	107.795	7.917
Gly56HA-N-NH	3.879	107.795	7.917
Gly57NH-N-NH	8.114	108.636	8.127
Gly57HA2-N-NH	3.943	108.639	8.127
Gly57HA3-N-NH	3.565	108.670	8.122
Ala58aNH-N-NH	7.937	129.129	7.949
Ala58aHA-N-NH	4.190	129.147	7.948
Ala58aHB-N-NH	1.367	129.130	7.949
Ala58bNH-N-NH	8.026	129.229	8.051
Ala58bHA-N-NH	4.176	129.233	8.049
Ala58bHB-N-NH	1.382	129.228	8.050

1 on 06/02/2009

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate at 5 degrees Celsius, acquired on 06/02/2009

Assignment	w1	w2
Gly12N-NH	110.755	8.594
Lys15N-NH	119.976	8.164
Ala16N-NH	125.236	8.518
Arg17aN-NH	121.038	8.453
Arg17bN-NH	122.658	8.544
Ile18N-NH	119.872	8.217
Ile19N-NH	126.807	8.468
Arg20N-NH	126.682	8.373
Tyr21N-NH	115.357	9.057
Phe22N-NH	119.361	9.709
Tyr23N-NH	123.151	9.708
Asn24N-NH	127.715	8.089
Ala25N-NH	127.026	8.576
Lys26N-NH	117.525	8.023
Ala27N-NH	118.636	7.012
Gly28N-NH	107.703	8.232
Leu29N-NH	115.073	6.991
Cys30aN-NH	119.165	8.919
Gln31N-NH	122.550	9.024
Thr32N-NH	110.296	8.289
Phe33N-NH	118.844	8.641
Val34N-NH	120.659	8.506
Tyr35N-NH	129.100	8.761
Gly36N-NH	109.058	8.367
Gly37N-NH	114.758	8.312
Ser38N-NH	115.701	8.366
Arg39N-NH	121.096	8.366
Ala40N-NH	123.874	8.215
Lys41N-NH	123.878	8.922
Arg42N-NH	120.224	8.113
Asn43N-NH	119.841	8.657
Asn44N-NH	117.769	7.963
Phe45N-NH	117.061	9.293
Lys46N-NH	120.163	9.946
Ser47N-NH	109.444	7.499
Ala48N-NH	125.362	8.318
Glu49N-NH	117.595	8.743
Asp50N-NH	119.813	7.913
Cys51N-NH	118.549	7.100
Met52N-NH	121.269	8.658
Arg53N-NH	120.040	7.974
Thr54N-NH	111.834	7.559
Ser55N-NH	115.480	7.755
Gly56N-NH	108.128	7.915
Gly57N-NH	108.633	8.123
Ala58aN-NH	128.862	7.941
Ala58bN-NH	129.062	8.038

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate at 20 degrees Celsius, acquired on 06/02/2009

Assignment	w1	w2
Gly12N-NH	110.738	8.506
Lys15N-NH	119.713	8.058
Ala16N-NH	124.965	8.384
Arg17N-NH	120.867	8.340
Ile18N-NH	119.819	8.104
Ile19N-NH	126.865	8.437
Arg20N-NH	126.528	8.332
Tyr21N-NH	115.659	8.997
Phe22N-NH	119.593	9.677
Asn24N-NH	127.754	8.081
Ala25N-NH	127.210	8.494
Lys26N-NH	117.469	7.964
Ala27N-NH	118.729	6.974
Gly28N-NH	107.669	8.194
Leu29N-NH	115.118	6.963
Cys30aN-NH	119.303	8.827
Cys30bN-NH	119.023	8.755
Gln31N-NH	122.732	8.988
Thr32N-NH	110.347	8.214
Phe33N-NH	118.816	8.569
Val34N-NH	120.734	8.408
Gly36N-NH	109.026	8.296
Gly37N-NH	114.355	8.256
Ser38N-NH	115.689	8.277
Arg39N-NH	121.134	8.278
Ala40N-NH	123.861	8.118
Lys41N-NH	123.669	8.806
Asn43N-NH	119.658	8.555
Asn44N-NH	119.346	7.946
Phe45N-NH	123.415	8.745
Ala48N-NH	125.543	8.278
Glu49N-NH	117.778	8.698
Asp50N-NH	119.684	7.845
Cys51N-NH	118.506	7.068
Met52N-NH	121.159	8.589
Arg53N-NH	119.927	7.956
Thr54N-NH	112.119	7.521
Ser55N-NH	115.676	7.722
Gly56N-NH	108.222	7.875
Gly57N-NH	108.742	8.064
Ala58aN-NH	128.994	7.856
Ala58bN-NH	129.157	7.937

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate at 36 degrees Celsius, acquired on 06/02/2009

Assignment	w1	w2
Lys15N-NH	119.710	7.995
Ala16N-NH	124.573	8.251
Arg17N-NH	120.571	8.227
Gly28N-NH	107.626	8.152
Cys30bN-NH	119.088	8.625
Phe33N-NH	118.781	8.480
Arg39N-NH	121.211	8.184
Ala40N-NH	123.757	8.037
Asn44N-NH	119.428	7.891
Phe45N-NH	123.424	8.658
Arg53N-NH	120.034	7.957
Thr54N-NH	111.908	7.442
Ala58aN-NH	129.151	7.785
Ala58bN-NH	129.285	7.832

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate in the presence of PDI, at a BPTI:PDI ratio 10:

Assignment	w1	w2
Gly12N-NH	110.796	8.611
Arg17N-NH	121.187	8.444
Ile18N-NH	119.874	8.228
Ala25N-NH	126.994	8.578
Lys26N-NH	117.478	8.025
Ala27N-NH	118.782	7.017
Gly28N-NH	107.661	8.242
Val34N-NH	121.109	8.489
Gly36N-NH	109.072	8.374
Gly37N-NH	114.529	8.367
Ser38N-NH	115.645	8.368
Arg39N-NH	121.073	8.370
Ala40N-NH	123.767	8.223
Arg42N-NH	120.182	8.131
Asn43N-NH	119.877	8.670
Phe45N-NH	123.436	8.822
Glu49N-NH	117.626	8.751
Met52N-NH	121.172	8.646
Arg53N-NH	120.035	7.980
Thr54N-NH	111.847	7.562
Ser55N-NH	115.559	7.759
Gly56N-NH	108.125	7.914
Gly57N-NH	108.644	8.127
Ala58aN-NH	128.856	7.941
Ala58bN-NH	129.079	8.043

1, acquired on 19/03/2009

Assignments for HSQC of (30-51, 5-14) BPTI Intermediate in the presence of PDI, at a BPTI:PDI ratio 50:

Assignment	w1	w2
Gly12N-NH	110.754	8.590
Lys15N-NH	120.089	8.163
Ala16N-NH	125.259	8.520
Arg17N-NH	121.049	8.457
Ile18N-NH	119.878	8.223
Ile19N-NH	126.875	8.465
Arg20N-NH	126.710	8.375
Tyr21N-NH	115.346	9.067
Phe22N-NH	119.387	9.711
Tyr23N-NH	123.170	9.707
Asn24N-NH	127.800	8.094
Ala25N-NH	127.044	8.579
Lys26N-NH	117.455	8.020
Ala27N-NH	118.661	7.010
Gly28N-NH	107.651	8.231
Leu29N-NH	115.041	6.986
Cys30N-NH	119.110	8.921
Gln31N-NH	122.562	9.028
Thr32N-NH	110.282	8.295
Phe33N-NH	118.840	8.648
Val34N-NH	120.644	8.503
Gly36N-NH	109.042	8.368
Gly37N-NH	114.741	8.320
Ser38N-NH	115.638	8.362
Arg39N-NH	121.144	8.361
Ala40N-NH	123.864	8.215
Lys41N-NH	123.874	8.922
Arg42N-NH	120.181	8.120
Asn43N-NH	119.828	8.665
Asn44N-NH	119.244	7.988
Phe45N-NH	123.409	8.820
Lys46N-NH	120.151	9.940
Ser47N-NH	109.454	7.498
Ala48N-NH	125.333	8.320
Glu49N-NH	117.576	8.747
Asp50N-NH	119.789	7.915
Cys51N-NH	118.637	7.097
Met52N-NH	121.233	8.657
Arg53N-NH	120.048	7.965
Thr54N-NH	111.829	7.554
Ser55N-NH	115.479	7.761
Gly56N-NH	108.098	7.917
Gly57N-NH	108.630	8.124
Ala58aN-NH	128.852	7.940
Ala58bN-NH	129.085	8.040

1, acquired on 19/03/2009

Assignments for 1H-1H TOCSY of recombinant wild type BPTI, acquired on 24/11/2008

Assignment	w1	w2
ASP3NH-NH	8.700	8.700
ASP3HA-NH	4.250	8.700
ASP3HB2-NH	2.759	8.689
PHE4NH-NH	7.780	7.779
PHE4HA-NH	4.591	7.777
PHE4HB2-NH	3.347	7.779
CYS5NH-NH	7.510	7.508
CYS5HA-NH	4.354	7.509
CYS5HB2-NH	2.843	7.509
CYS5HB3-NH	2.770	7.509
LEU6NH-NH	7.573	7.568
LEU6HA-NH	4.512	7.568
LEU6HB2-NH	1.839	7.568
LEU6HB3-NH	1.683	7.567
GLU7NH-NH	7.528	7.527
GLU7HA-NH	4.586	7.528
GLU7HB2-NH	2.257	7.529
GLU7HB3-NH	2.165	7.529
GLU7HG-NH	2.569	7.529
TYR10NH-NH	7.804	7.801
TYR10HA-NH	4.930	7.802
TYR10HB2-NH	2.955	7.802
THR11NH-NH	8.956	8.951
THR11HA-NH	4.527	8.952
THR11HB-NH	4.048	8.951
THR11HG-NH	1.387	8.955
GLY12NH-NH	7.163	7.158
GLY12HA2-NH	3.895	7.159
GLY12HA3-NH	3.260	7.159
CYS14NH-NH	8.716	8.692
CYS14HA-NH	4.558	8.692
CYS14HB2-NH	3.461	8.692
CYS14HB3-NH	2.798	8.692
LYS15NH-NH	7.966	7.966
LYS15HA-NH	4.407	7.972
LYS15HB2-NH	2.085	7.966
LYS15HB3-NH	1.575	7.968
ALA16NH-NH	8.216	8.214
ALA16HA-NH	4.296	8.202
ALA16HB-NH	1.171	8.210
ARG17NH-NH	8.195	8.189
ARG17HA-NH	4.312	8.189
ARG17HB2-NH	1.594	8.189
ARG17HB3-NH	1.476	8.189
ARG17HG2-NH	1.303	8.189
ILE18NH-NH	8.118	8.115
ILE18HA-NH	4.195	8.116
ILE18HB-NH	1.867	8.115
ILE18HG2-NH	0.963	8.115
ILE19NH-NH	8.690	8.689
ILE19HA-NH	4.307	8.688
ILE19HB-NH	1.947	8.688

ARG20NH-NH	8.397	8.394
ARG20HA-NH	4.697	8.392
ARG20HB2-NH	1.807	8.395
ARG20HB3-NH	0.812	8.395
TYR21NH-NH	9.187	9.186
TYR21HA-NH	5.679	9.186
TYR21HB2-NH	2.700	9.187
PHE22NH-NH	9.778	9.776
PHE22HA-NH	5.271	9.776
PHE22HB2-NH	2.906	9.777
PHE22HB3-NH	2.816	9.776
TYR23NH-NH	10.568	10.567
TYR23HA-NH	4.297	10.568
TYR23HB2-NH	3.463	10.567
TYR23HB3-NH	2.738	10.569
ASN24NH-NH	7.864	7.757
ASN24HA-NH	4.603	7.757
ASN24HB2-NH	2.862	7.758
ASN24HB3-NH	2.169	7.757
ALA25NH-NH	8.791	8.789
ALA25HA-NH	3.760	8.789
ALA25HB-NH	1.554	8.788
LYS26NH-NH	7.913	7.913
LYS26HA-NH	4.067	7.912
LYS26HB2-NH	1.884	7.912
ALA27NH-NH	6.819	6.817
ALA27HA-NH	4.292	6.816
ALA27HB-NH	1.184	6.816
GLY28NH-NH	8.148	8.145
GLY28HA2-NH	3.919	8.140
GLY28HA3-NH	3.628	8.140
LEU29NH-NH	6.830	6.828
LEU29HA-NH	4.755	6.828
LEU29HB2-NH	1.730	6.828
LEU29HB3-NH	1.429	6.828
CYS30NH-NH	8.406	8.406
CYS30HA-NH	5.607	8.405
CYS30HB2-NH	3.672	8.405
CYS30HB3-NH	2.665	8.406
GLN31NH-NH	8.766	8.763
GLN31HA-NH	4.824	8.763
GLN31HB2-NH	2.223	8.763
GLN31HB3-NH	1.729	8.763
THR32NH-NH	8.038	8.036
THR32HA-NH	5.291	8.036
THR32HB-NH	4.035	8.031
PHE33NH-NH	9.374	9.375
PHE33HA-NH	4.867	9.375
PHE33HB2-NH	3.088	9.375
PHE33HB3-NH	2.949	9.375
VAL34NH-NH	8.368	8.368
VAL34HA-NH	3.915	8.367
VAL34HB-NH	1.947	8.368
TYR35NH-NH	9.389	9.387
TYR35HA-NH	4.874	9.388
TYR35HB2-NH	2.664	9.387

TYR35HB3-NH	2.501	9.388
GLY36NH-NH	8.640	8.609
GLY36HA2-NH	4.317	8.608
GLY36HA3-NH	3.241	8.607
GLY37NH-NH	4.302	4.301
GLY37HA2-NH	4.219	4.315
GLY37HA3-NH	2.903	4.311
CYS38NH-NH	7.754	7.755
CYS38HA-NH	4.951	7.755
CYS38HB2-NH	3.955	7.755
CYS38HB3-NH	3.029	7.755
ARG39NH-NH	9.073	9.074
ARG39HA-NH	3.937	9.075
ARG39HB2-NH	2.271	9.076
ARG39HB3-NH	1.594	9.075
ALA40NH-NH	7.422	7.425
ALA40HA-NH	4.080	7.420
ALA40HB-NH	1.200	7.420
LYS41NH-NH	8.338	8.331
LYS41HA-NH	4.439	8.325
LYS41HA-NH	4.439	8.329
LYS41HB2-NH	2.251	8.331
LYS41HB3-NH	1.657	8.331
ARG42NH-NH	8.361	8.357
ARG42HA-NH	3.658	8.359
ARG42HB2-NH	1.014	8.357
ARG42HB3-NH	0.341	8.357
ASN43NH-NH	7.224	7.225
ASN43HA-NH	5.052	7.204
ASN43HB2-NH	3.335	7.204
ASN43HB3-NH	3.285	7.204
ASN44NH-NH	6.759	6.762
ASN44HA-NH	4.898	6.763
ASN44HB2-NH	2.775	6.763
ASN44HB3-NH	2.503	6.763
PHE45NH-NH	9.937	9.938
PHE45HA-NH	5.125	9.939
PHE45HB2-NH	3.406	9.939
PHE45HB3-NH	2.787	9.939
LYS46NH-NH	9.909	9.909
LYS46HA-NH	4.383	9.909
LYS46HB2-NH	2.092	9.917
LYS46HB3-NH	1.983	9.922
SER47NH-NH	7.467	7.466
SER47HA-NH	4.531	7.466
SER47HB2-NH	4.124	7.466
SER47HB3-NH	3.862	7.466
ALA48NH-NH	8.138	8.140
ALA48HA-NH	3.155	8.145
ALA48HB-NH	1.035	8.139
GLU49NH-NH	8.603	8.603
GLU49HA-NH	3.858	8.603
GLU49HB2-NH	2.005	8.603
GLU49HB3-NH	1.834	8.603
GLU49HG2-NH	2.334	8.603
GLU49HG3-NH	2.184	8.603

ASP50NH-NH	7.852	7.851
ASP50HA-NH	4.281	7.837
ASP50HB2-NH	2.870	7.851
ASP50HB2-NH	2.870	7.854
ASP50HB3-NH	2.719	7.851
CYS51NH-NH	6.989	6.984
CYS51HA-NH	1.687	6.984
CYS51HB2-NH	3.175	6.985
CYS51HB3-NH	2.892	6.984
MET52NH-NH	8.585	8.582
MET52HA-NH	4.170	8.581
MET52HB2-NH	2.052	8.580
MET52HB3-NH	1.963	8.581
MET52HG-NH	2.692	8.579
ARG53NH-NH	8.268	8.267
ARG53HA-NH	3.986	8.266
ARG53HB2-NH	1.918	8.266
ARG53HB3-NH	1.869	8.266
THR54NH-NH	7.401	7.397
THR54HA-NH	4.078	7.397
THR54HB-NH	4.005	7.397
THR54HG-NH	1.615	7.397
CYS55NH-NH	8.201	8.205
CYS55HA-NH	4.643	8.205
CYS55HB2-NH	2.221	8.204
CYS55HB3-NH	2.024	8.205
GLY56NH-NH	8.000	8.000
GLY56HA2-NH	3.848	7.990
GLY57NH-NH	8.211	8.212
GLY57HA2-NH	3.950	8.211
GLY57HA3-NH	3.842	8.211
ALA58NH-NH	7.920	7.919
ALA58HA-NH	4.025	7.919
ALA58HB-NH	1.303	7.917

Assignments for HSQC of Wild Type BPTI at 5 degrees Celsius, acquired on 19/03/2009

Assignment	w1	w2
Asp3N-NH	123.630	8.764
Phe4N-NH	117.510	8.060
Cys5N-NH	121.612	7.609
Leu6N-NH	113.719	7.700
Glu7N-NH	120.326	7.587
Tyr10N-NH	123.596	7.971
Thr11N-NH	127.620	9.203
Gly12N-NH	107.590	7.347
Cys14N-NH	120.471	8.844
Lys15N-NH	115.610	8.145
Ala16N-NH	123.711	8.287
Arg17N-NH	118.742	8.449
Ile18N-NH	125.958	8.262
Ile19N-NH	128.352	8.927
Arg20N-NH	130.263	8.495
Tyr21N-NH	115.202	9.307
Phe22N-NH	119.902	9.863
Tyr23N-NH	124.867	10.702
Asn24N-NH	125.282	7.773
Ala25N-NH	126.191	9.043
Lys26N-NH	117.459	8.109
Ala27N-NH	118.658	6.917
Gly28N-NH	107.326	8.265
Leu29N-NH	114.922	6.938
Cys30N-NH	118.304	8.580
Gln31N-NH	122.928	8.856
Thr32N-NH	108.526	8.198
Phe33N-NH	119.153	9.461
Val34N-NH	118.848	8.590
Tyr35N-NH	129.711	9.568
Gly36N-NH	114.361	8.766
Cys38N-NH	115.000	7.804
Arg39N-NH	113.264	9.285
Ala40N-NH	118.225	7.553
Lys41N-NH	121.204	8.464
Arg42N-NH	116.143	8.565
Asn43N-NH	116.159	7.277
Asn44N-NH	120.730	6.856
Phe45N-NH	122.714	10.054
Lys46N-NH	120.370	10.139
Ser47N-NH	108.942	7.541
Ala48N-NH	125.414	8.297
Glu49N-NH	117.583	8.721
Asp50N-NH	120.698	8.019
Cys51N-NH	119.771	7.073
Met52N-NH	120.550	8.687
Arg53N-NH	122.057	8.333
Thr54N-NH	113.427	7.493
Cys55N-NH	115.027	8.388
Gly56N-NH	108.082	8.203
Gly57N-NH	109.635	8.459
Ala58N-NH	128.702	8.026

Assignment	w1	w2
ASP3N-NH	123.360	8.509
PHE4N-NH	117.015	7.780
CYS5N-NH	121.564	7.428
LEU6N-NH	114.008	7.503
GLU7N-NH	120.645	7.436
TYR10N-NH	123.573	7.758
THR11N-NH	127.581	8.924
GLY12N-NH	107.517	7.110
CYS14N-NH	120.312	8.645
LYS15N-NH	115.778	7.922
ALA16N-NH	123.796	8.130
ARG17N-NH	118.744	8.173
ILE18N-NH	125.966	8.067
ILE19N-NH	128.452	8.662
ARG20N-NH	130.181	8.314
TYR21N-NH	115.489	9.124
PHE22N-NH	120.056	9.699
TYR23N-NH	125.050	10.506
ASN24N-NH	125.474	7.650
ALA25N-NH	126.478	8.769
LYS26N-NH	117.350	7.854
ALA27N-NH	118.744	6.740
GLY28N-NH	107.295	8.074
LEU29N-NH	114.957	6.754
CYS30N-NH	118.578	8.353
GLN31N-NH	123.126	8.689
THR32N-NH	108.653	7.982
PHE33N-NH	119.310	9.297
VAL34N-NH	118.956	8.330
TYR35N-NH	129.866	9.345
GLY36N-NH	114.431	8.553
CYS38N-NH	115.214	7.656
ARG39N-NH	113.597	9.058
ALA40N-NH	118.335	7.361
LYS41N-NH	121.293	8.268
ARG42N-NH	116.067	8.323
ASN43N-NH	116.296	7.118
ASN44N-NH	120.972	6.690
PHE45N-NH	122.787	9.865
LYS46N-NH	120.610	9.892
SER47N-NH	109.027	7.387
ALA48N-NH	125.591	8.097
GLU49N-NH	117.800	8.533
ASP50N-NH	120.586	7.796
CYS51N-NH	119.886	6.899
MET52N-NH	120.855	8.495
ARG53N-NH	121.704	8.183
THR54N-NH	113.506	7.325
CYS55N-NH	115.029	8.156
GLY56N-NH	108.018	7.942
GLY57N-NH	109.541	8.194
ALA58N-NH	128.895	7.754

Assignments for HSQC of Wild Type BPTI in the presence of PDI, at a BPTI:PDI ratio 1:1, acquired on 19

Assignment	w1	w2
Asp3N-NH	123.725	8.758
Gly57N-NH	109.616	8.464
Ala58N-NH	128.692	8.027

3/03/2009