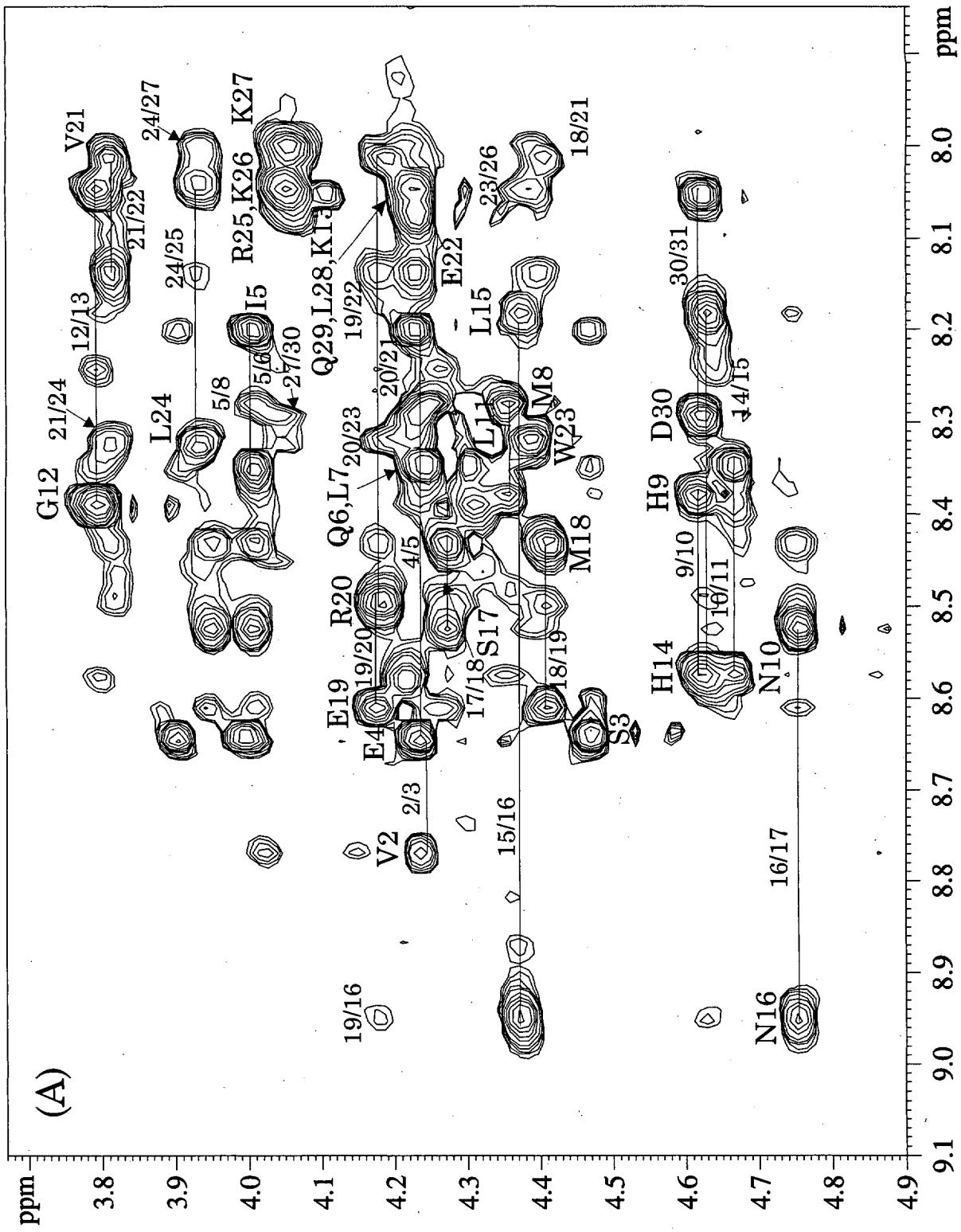
Table S1. Proton resonance assignment of the hPTP(1-31)NH_2 peptide in aqueous solution at pH 6.8 and at 5 °C

	NH	CαH	CβHs	Others
Ser-1	----	4.25	4.04, 4.02	
Val-2	8.78	4.18	2.14	CγH$_3$#: 1.00
Ser-3	8.65	4.42	3.91, 4.00	
Glu-4	8.65	4.17	2.09, 2.03	CγHs 2.34, 2.28
Ile-5	8.21	3.96	1.86	CγHs 1.55, 1.23, CH$_3$#: 0.90
Gln-6	8.36	4.19	2.10#	CγHs#: 2.41, CεH 7.68, 7.05
Leu-7	8.35	4.19	1.72, 1.58	CγHs# 1.66, CδH$_3$s: 0.93, 0.89
Met-8	8.29	4.30	2.06#	CγHs 2.52, 2.63
His-9	8.39	4.57	3.26, 3.18	Cδ2H 7.20, Cε1H 8.30
Asn-10	8.58	4.62	2.85, 2.91	NδHs 7.77, 7.09
Leu-11	8.36	4.26	1.76, 1.70	CγHs# 1.63, CδH$_3$s 0.93, 0.88
Gly-12	8.40	3.75#		
Lys-13	8.06	4.17	1.73#,	CγHs 1.37, 1.31, CδHs# 1.65, CεHs# 2.98
His-14	8.59	4.59	3.21, 3.14	Cδ2H 7.16, Cε1H 8.25
Leu-15	8.19	4.32	1.61, 1.50,	CγHs# 1.44, CδH$_3$s 0.77, 0.74
Asn-16	8.95	4.71	3.06, 2.91,	NδHs 7.07, 7.72
Ser-17	8.53	4.22	3.96, 4.01	
Met-18	8.44	4.36	2.16#,	CγHs 2.60, 2.70
Glu-19	8.62	4.12	2.05, 2.12	CγHs: 2.30, 2.46
Arg-20	8.50	4.15	1.87, 1.98	CγHs 1.65, 1.73, CδHs# 3.21, NεH 7.32, NηHs# 6.90, 6.60
Val-21	8.02	3.76	2.21,	CγH$_3$s: 1.11, 0.97
Glu-22	8.15	4.17	2.11,	CγHs#: 2.37
Trp-23	8.33	4.34	3.35, 3.47	Cδ1H: 7.28, Nε1H: 10.28, Cε3H: 7.59,
Leu-24	8.34	3.88	1.83#	CγH 1.60, CδH$_3$s# 0.96
Arg-25	8.05	4.02	1.59, 1.75	CγHs 1.91, 1.95, CδHs 3.18, 3.24, NεH 7.59, NηHs 7.01, 6.75
Lys-26	8.06	4.05	1.67#	CγHs 1.80, 1.85, CδHs 1.41, 1.54, CεHs 2.99
Lys-27	8.01	3.99	1.55, 1.69	CγHs# 1.19, CδHs#: 1.47, CεHs 2.77, 2.86
Leu-28	8.06	4.18	1.73,	CγH 1.60, CδH$_3$s 0.94, 0.88
Gln-29	8.09	4.18	2.09, 2.14,	CγHs#: 2.43, NεHs 7.68, 6.99
Asp-30	8.30	4.57	2.67, 2.77	
Val-31	8.06	4.06	2.20,	CγH$_3$s#: 0.99

Degenerate proton resonances.

Figure S1. The fingerprint (NH-CαH) region of a NOESY spectrum of hPTH(1-31)NH_2 in aqueous solution at pH 6.8 and at a temperature of 5 °C. (A) the NOESY region showing sequential and some helix-indicating NOE connectivities. (B) a spectral region showing NH-NH NOE connectivities. The 'noise' band between 8.2 and 8.3 ppm is caused by the much sharper resonances of the ring CH protons of His14 and His9 relative to the broader backbone NH proton resonances in the peptide.

Fig S1A


(A)
ppm
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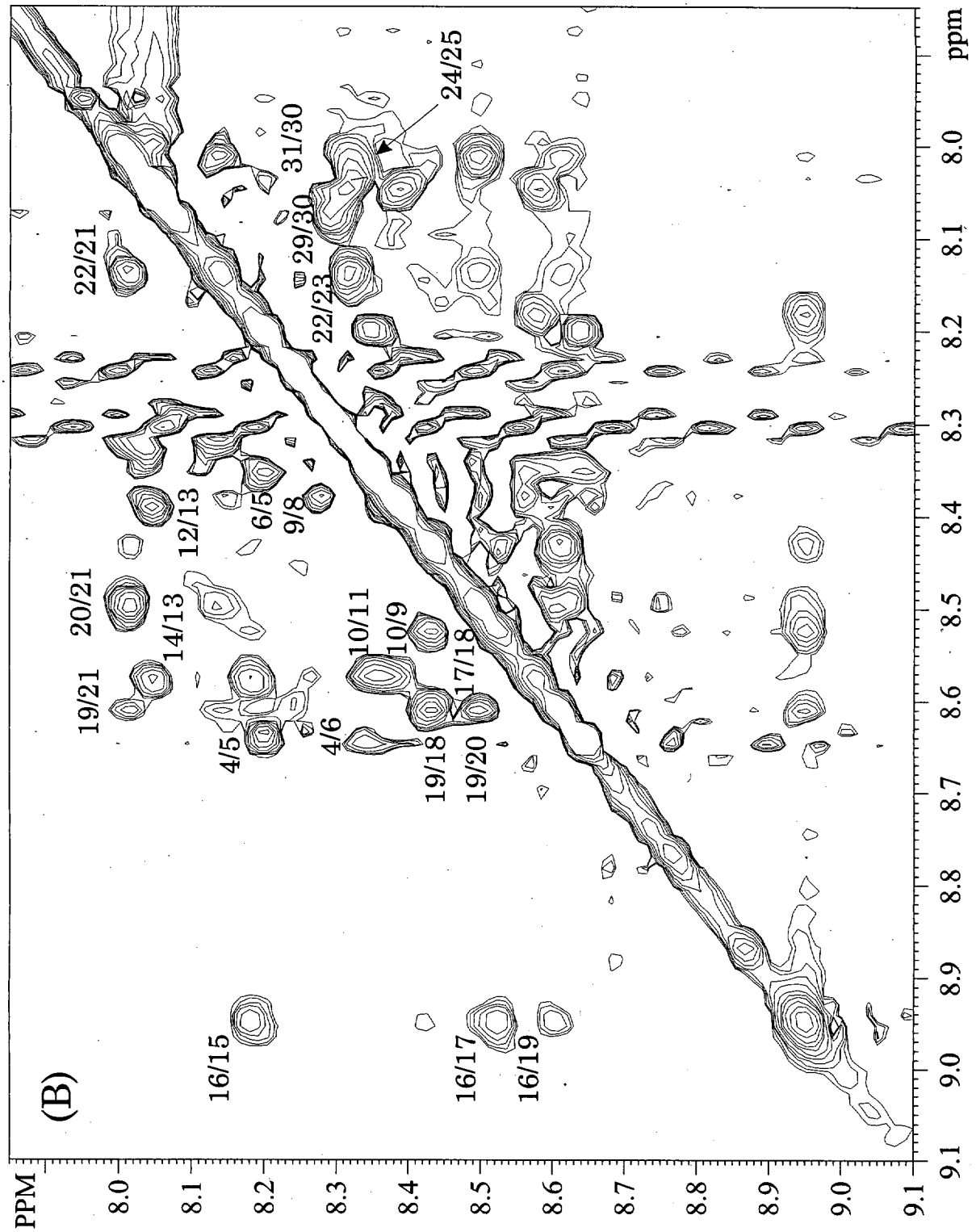
3.9
4.0
4.1
4.2
4.3
4.4
4.5
4.6
4.7
4.8
4.9
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
G12
21/24
V21
21/22
12/13
L24
24/25
24/27
5/8
I5
5/6
27/30
R25,K26
K27
Q29,L28,K1
19/22
20/23
20/21
Q6,L7
R20
4/5
E19
19/20
E4
2/3
V2
19/16
17/18
S17
15/16
E22
23/26
L15
L11
M8
W23
M18
18/19
S3
18/21
H14
9/10
10/11
N10
16/17
N16
H9
D30
30/31
14/15

Fig. S1B


(B)
PPM
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8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.8
8.9
9.0
9.1
22/21
31/30
24/25
29/30
22/23
12/13
6/5
9/8
20/21
14/13
19/21
4/5
4/6
10/11
10/9
17/18
19/18
19/20
16/15
16/17
16/19