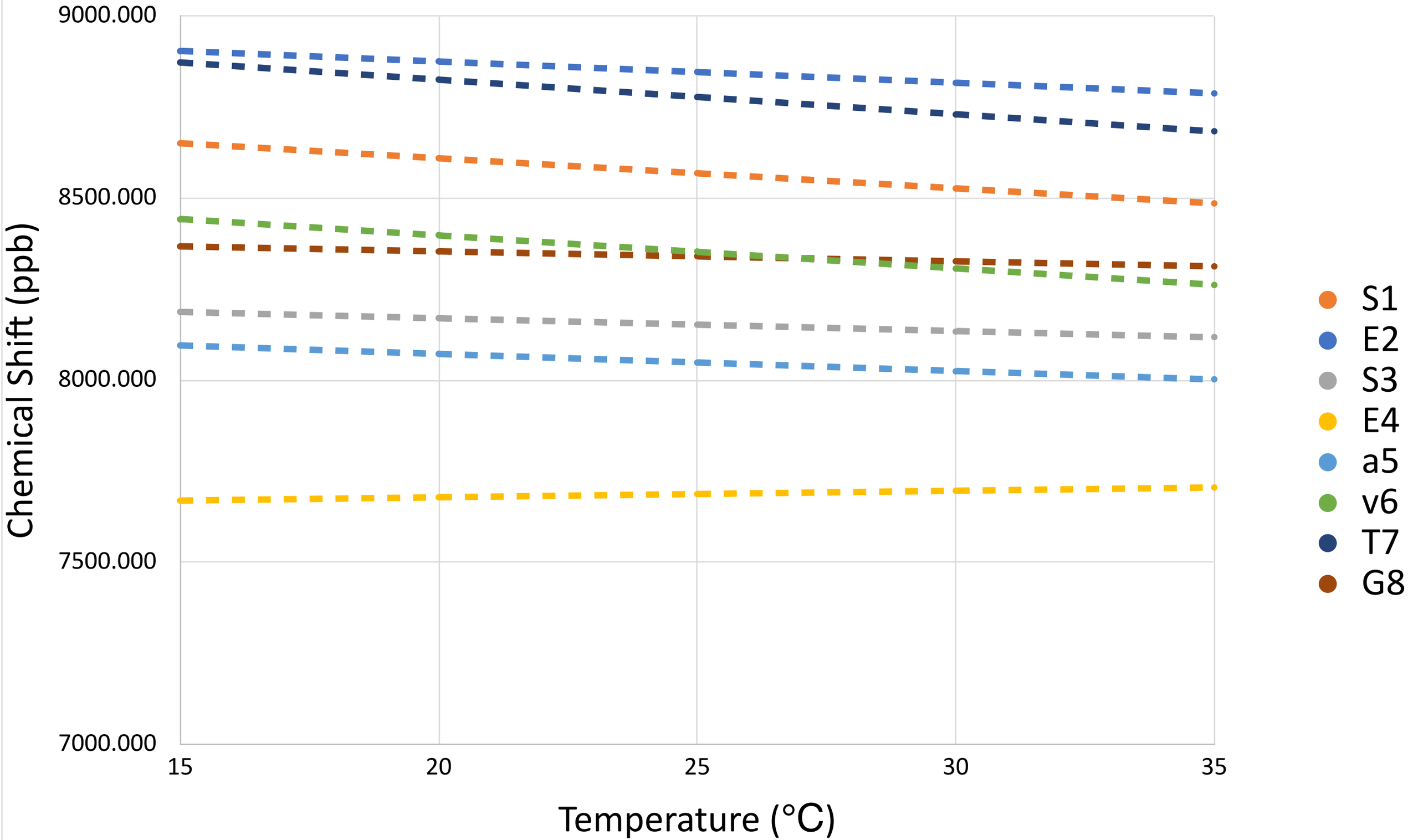
Residue	Slope (ppb/°C)
Ser1	-8.3
Glu2	-5.8
Ser3	-3.5
Glu4	1.8
D-Ala5	-4.7
D-Val6	-9
Thr7	-9.5
Gly8	-2.7

Chemical Shift vs. Temperature



NMR reveals hydrogen bond network in cyclo-(SESEavTG)

Residue	Slope (ppb/°C)	H-bond*
Glu4	1.8	Yes
Gly8	-2.7	Yes
Ser3	-3.5	Yes
D-Ala5	-4.7	No
Glu2	-5.8	No
Ser1	-8.3	No
D-Val6	-9	No
Thr7	-9.5	No

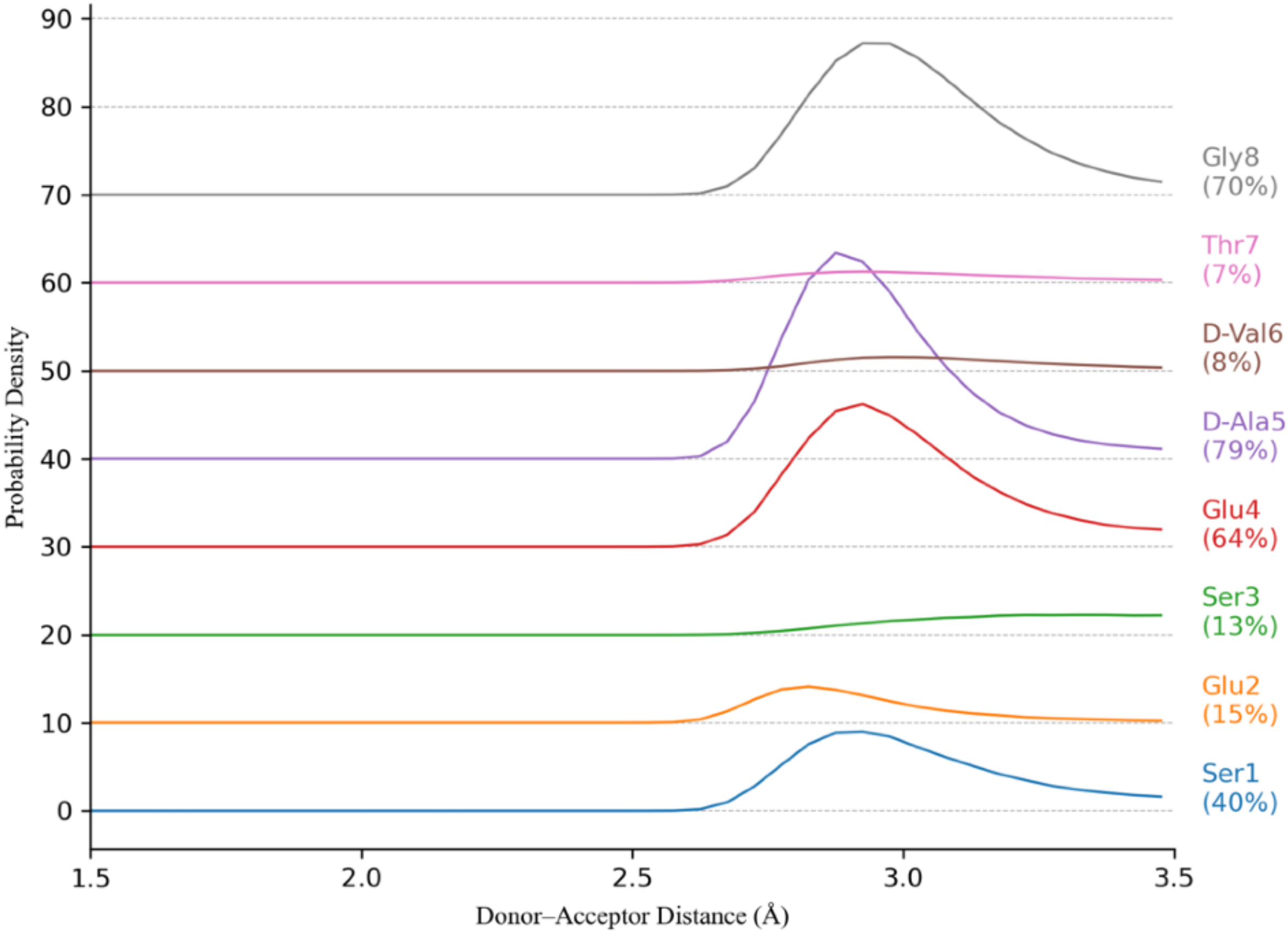
*using -4.5 ppb/°C as cutoff

Baxter, N. J. & Williamson, M. P., *J. Biomol. NMR* **9**, 359-369, (1997)

Residue	Slope (ppb/°C)	H-bond*
Glu4	1.8	Yes
Gly8	-2.7	Yes
Ser3	-3.5	Yes
D-Ala5	-4.7	No
Glu2	-5.8	No
Ser1	-8.3	No
D-Val6	-9	No
Thr7	-9.5	No

*using -4.5 ppb/°C as cutoff

Baxter, N. J. & Williamson, M. P., *J. Biomol. NMR* **9**, 359-369, (1997)


90
80
70
60
50
40
30
20
10
0
Probability Density
1.5
2.0
2.5
3.0
3.5
Donor–Acceptor Distance (Å)
Gly8
(70%)
Thr7
(7%)
D-Val6
(8%)
D-Ala5
(79%)
Glu4
(64%)
Ser3
(13%)
Glu2
(15%)
Ser1
(40%)

network aligns with experimental data

Simulation prediction of hydrogen bond

Residue	Slope (ppb/°C)	H-bond	Predicted H-bond*
Glu4	1.8	Yes	Yes
Gly8	-2.7	Yes	Yes
Ser3	-3.5	Yes	No
D-Ala5	-4.7	No	Yes
Glu2	-5.8	No	No
Ser1	-8.3	No	No
D-Val6	-9	No	No
Thr7	-9.5	No	No

*using 50% as the cutoff