## Thermal Melting Studies of Alkyne and Ferrocene-containing PNA Bioconjugates

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## I. UV-Vis spectra



**Figure 1.** UV/Vis spectrum of **1-ferrocenyl-4-propyl-1,2,3-triazole** (left) and linear plot of the absorbance at 260 nm against the concentration.



**Figure 2.** UV/Vis spectrum of **PNA1** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**1**, PNA alkyne monomer).



**Figure 3.** UV/Vis spectrum of **PNA3** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**1**, PNA alkyne monomer).



**Figure 4.** UV/Vis spectrum of **PNA5** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**1**, PNA alkyne monomer).



**Figure 5.** UV/Vis spectrum of **PNA7** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**1**, PNA alkyne monomer).



**Figure 6.** UV/Vis spectrum of **PNA2** (left), linear plot of the absorbance at 260 nm against the dilution (right) (**2**, PNA ferrocene monomer).



**Figure 7.** UV/Vis spectrum of **PNA6** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**2**, PNA ferrocene monomer).



**Figure 8.** UV/Vis spectrum of **PNA8** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**2**, PNA ferrocene monomer).



**Figure 9.** UV/Vis spectrum of **PNA4** (left) and linear plot of the absorbance at 260 nm against the dilution (right) (**2**, PNA ferrocene monomer).



Figure 10. PNA1-DNA1: polynomial fits of the heating (left) and cooling (right) curve of 9th degree (red) and its derivatives (blue) with local maxima as the melting temperatures  $T_m$  in cycle 1.



**Figure 11. PNA1-DNA1**: polynomial fits of the heating (left) and cooling (right) curve of 9th degree (red) and its derivatives (blue) with local maxima as the melting temperatures  $T_m$  in cycle 2.



Figure 12. UV/Vis melting spectrum of PNA3-DNA1.



Figure 13. UV/Vis melting spectrum of PNA5-DNA1.



Figure 14. UV/Vis melting spectrum of PNA7-DNA1.



Figure 15. UV/Vis melting spectrum of PNA1-DNA2.



80

90

Figure 16. UV/Vis melting spectrum of PNA3-DNA2.



Figure 17. UV/Vis melting spectrum of PNA5-DNA2.



Figure 18. UV/Vis melting spectrum of PNA7-DNA2.



Figure 19. UV/Vis melting spectrum of PNA2 and DNA1.



Figure 20. UV/Vis melting spectrum of PNA4 and DNA1.



Figure 21. UV/Vis melting spectrum of PNA6 and DNA1.



Figure 22. UV/Vis melting spectrum of PNA8 and DNA1.



Figure 23. UV/Vis melting spectrum of PNA2 and DNA2.



Figure 24. UV/Vis melting spectrum of PNA4 and DNA2.



Figure 25. UV/Vis melting spectrum of PNA6 and DNA2.



Figure 26. UV/Vis melting spectrum of PNA8 and DNA2.



Figure 27. UV/Vis melting spectrum of DNA1-cDNA1.



Figure 28. UV/Vis melting spectrum of DNA2-cDNA2.



Figure 29. UV/Vis melting spectrum of DNA1-cDNA2.



Figure 30. UV/Vis melting spectrum of DNA2-cDNA1.



Figure 31. UV/Vis melting spectrum of PNA5-DNA3.



Figure 32. UV/Vis melting spectrum of PNA5-DNA4.



Figure 33. UV/Vis melting spectrum of PNA5-DNA5.



Figure 34. UV/Vis melting spectrum of PNA6-DNA3.



Figure 35. UV/Vis melting spectrum of PNA6-DNA4.



Figure 36. UV/Vis melting spectrum of PNA6-DNA5.







Figure 38. UV/Vis melting spectrum of PNA5-DNA7.



Figure 39. UV/Vis melting spectrum of PNA5-DNA8.



Figure 40. UV/Vis melting spectrum of PNA5-DNA9.



Figure 41. UV/Vis melting spectrum of PNA6-DNA6.



Figure 42. UV/Vis melting spectrum of PNA6-DNA7.



Figure 43. UV/Vis melting spectrum of PNA6-DNA8.



Figure 44. UV/Vis melting spectrum of PNA6-DNA9.



Figure 45. UV/Vis melting spectrum of PNA9-DNA1.



Figure 46. UV/Vis melting spectrum of PNA9-DNA2.



Figure 47. UV/Vis melting spectrum of PNA10-DNA1.



Figure 48. UV/Vis melting spectrum of PNA10-DNA2.



Figure 49. MALDI mass spectrum of PNA9: 3097.6 m/z. Expected 3096.99 m/z.



Figure 50. MALDI mass spectrum of PNA10: 3039.3 m/z. Expected 3039.94 m/z.



Figure 51. CD spectra of alkyne and ferrocene-containing PNA-DNA hybrids.