Supplementary Material (ESI) for Chemical Communications

Effect of chirality of L/D-proline and prochiral glycine as the linker amino acid in 5-atom linked Thymidinyl-(α-amino acid)-Thymidine dimers

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Mass and ^{1}H NMR for compound **Ia**

Mass and ^{1}H NMR for compound **Ib**

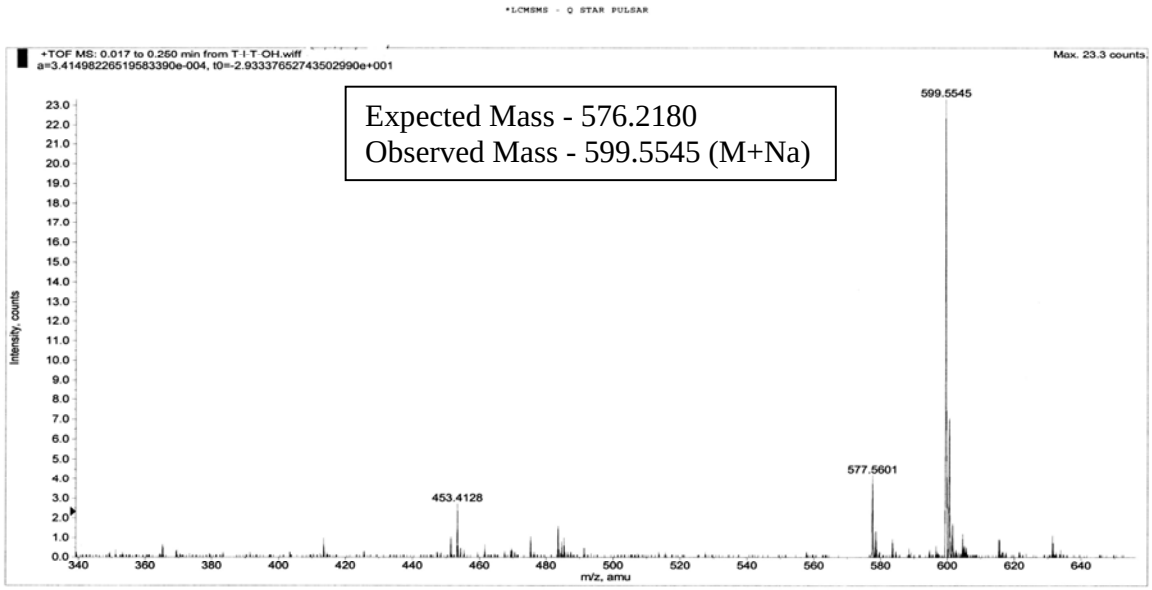
Mass and ^{1}H NMR for compound **Ic**

N↔S sugar conformation preferences in **Ia**, **Ib** & **Ic**

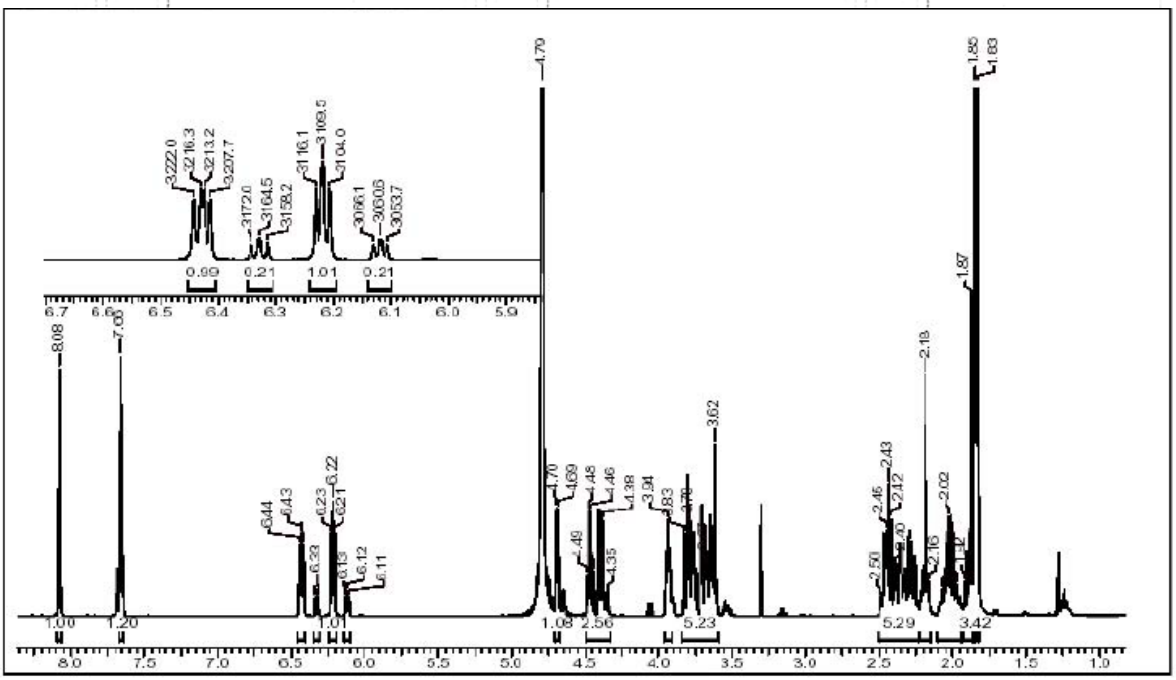
2D-COSY ^{1}H NMR for compound **Ic**

Temperature dependent ^{1}H-NMR shift in H-6 proton of compound **Ib**

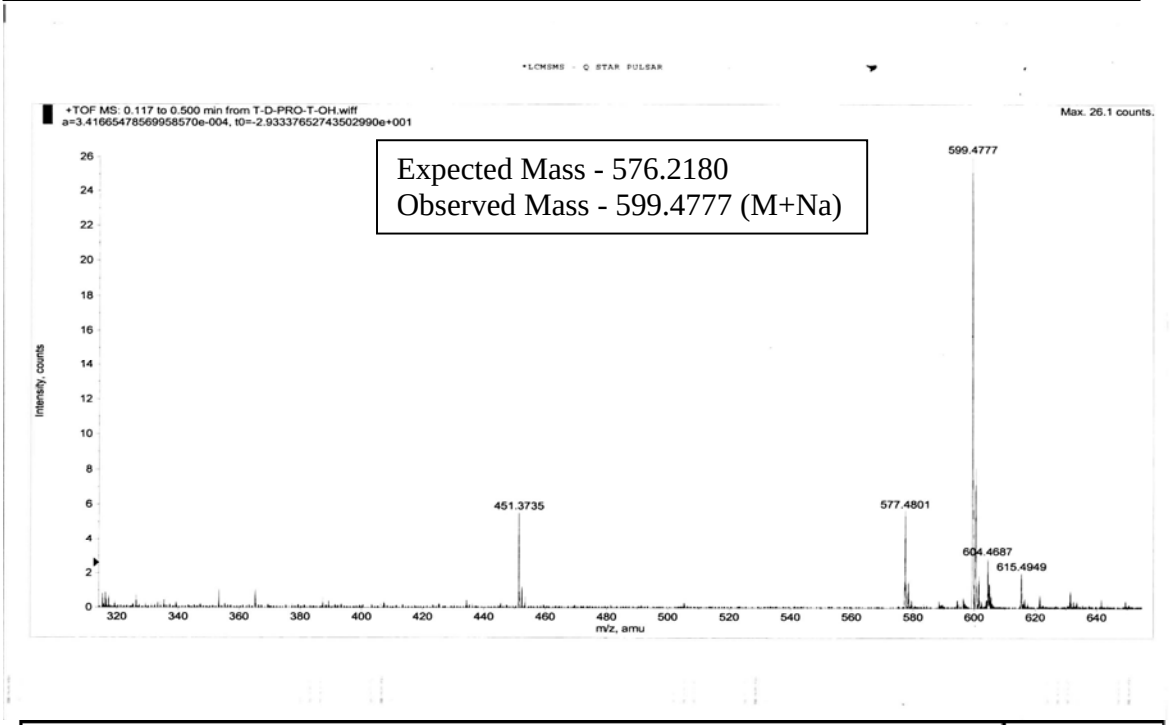
Compound Ia Mass and ^{1}H NMR



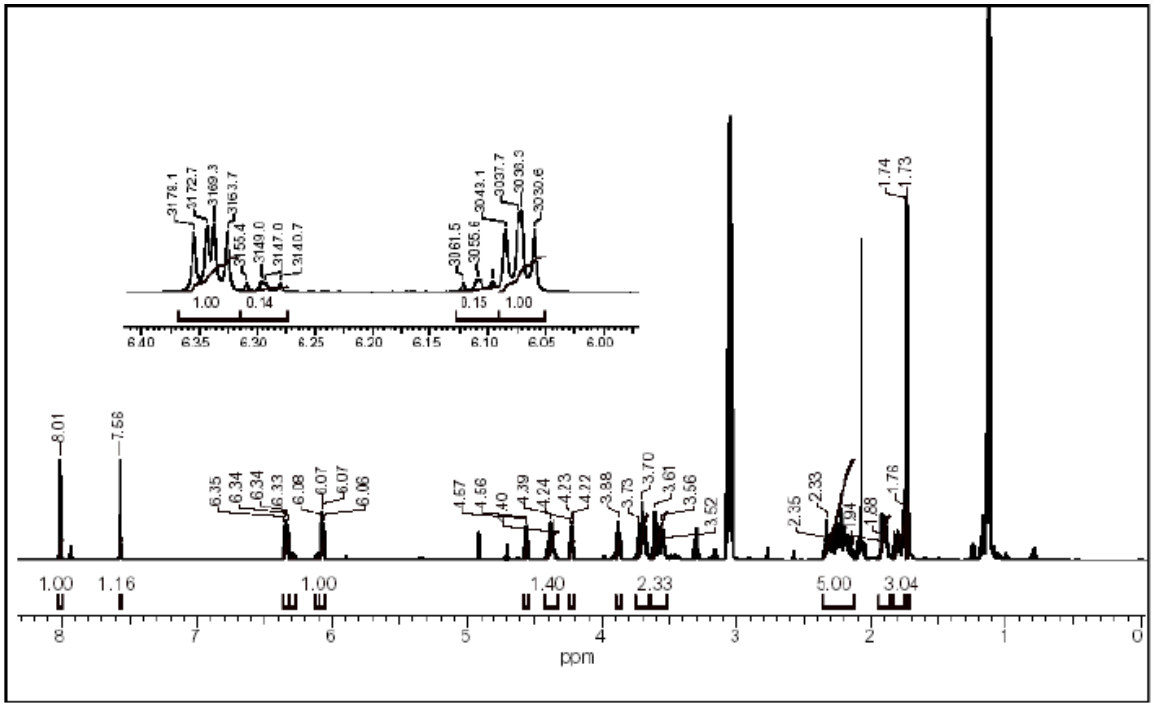
Expected Mass - 576.2180
Observed Mass - 599.5545 (M+Na)



Compound **Ib** Mass and ^{1}H NMR



Expected Mass - 576.2180
Observed Mass - 599.4777 (M+Na)



Compound **Ic** Mass and ^{1}H NMR

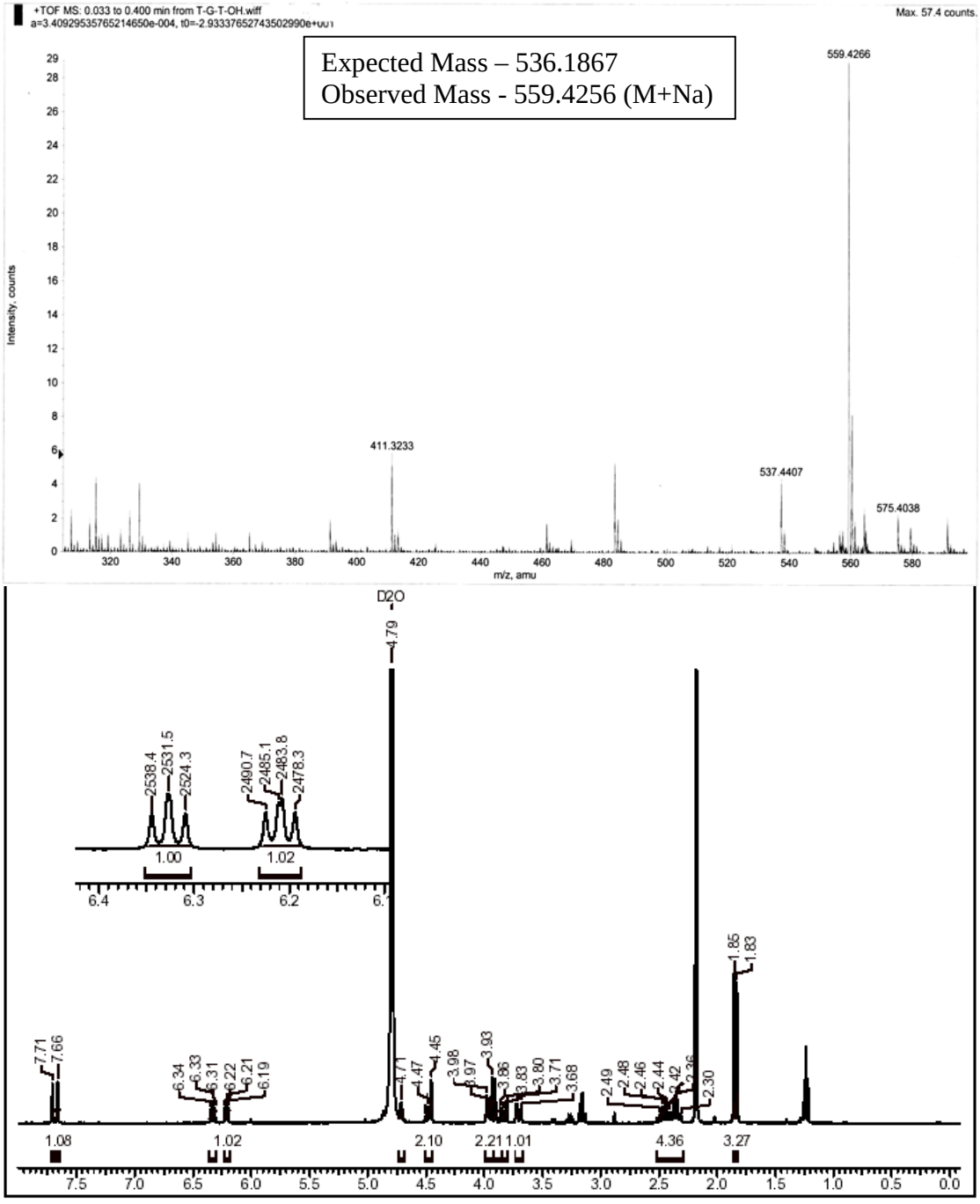
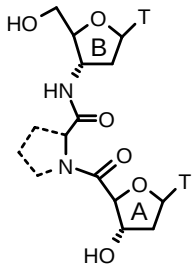
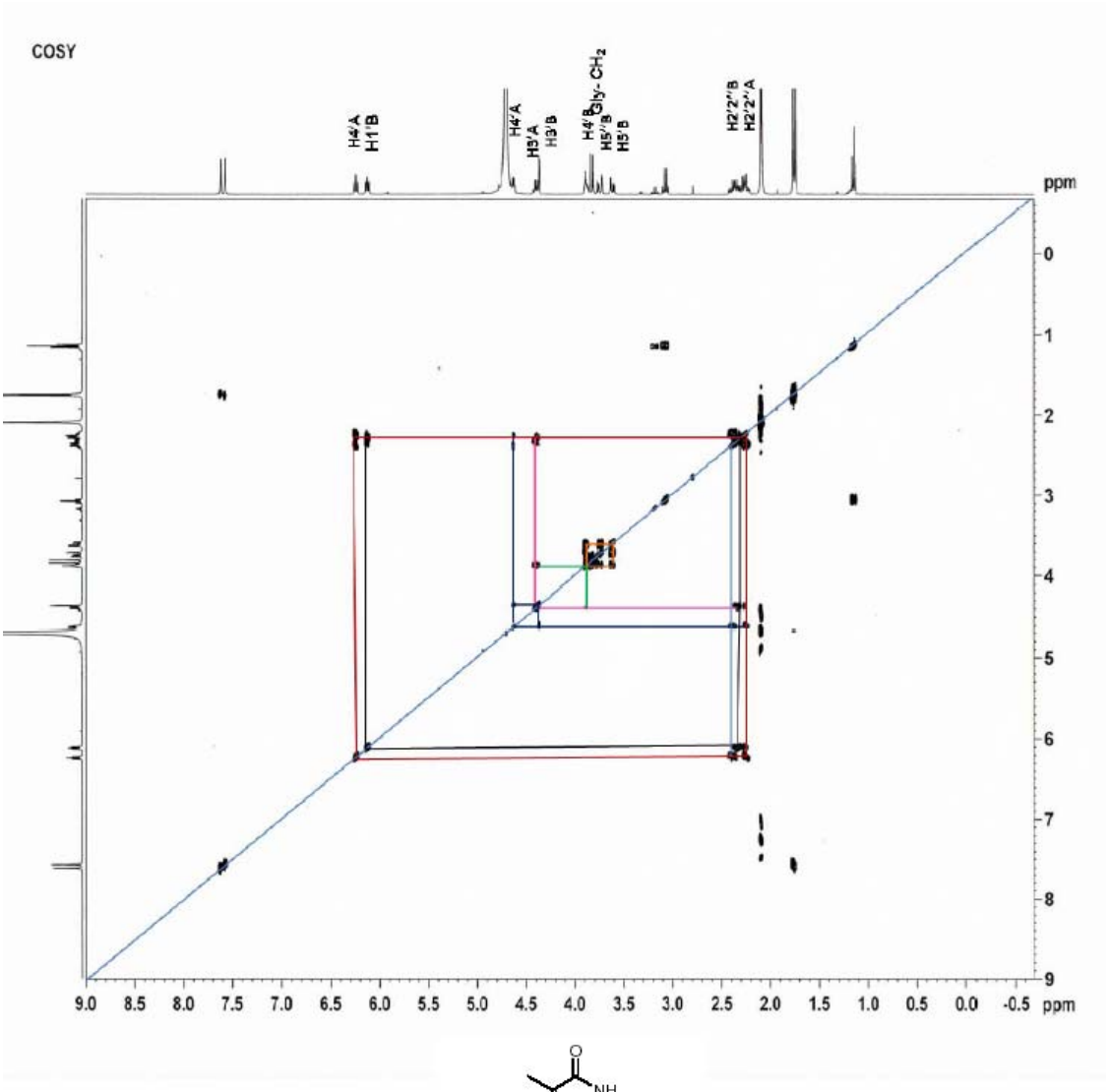


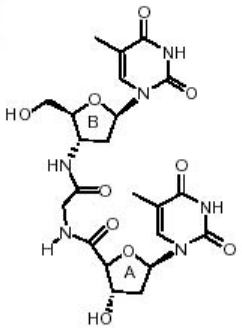
Table 1. N↔S sugar conformation preferences in T-(amino acid)-T dimers **Ia**, **Ib** & **Ic**

Compound		$J_{H1',H2'}$ **(Hz)**	$J_{H1',H2''}$ **(Hz)**	**%S**	**%N**	
Ia[#]	Ring A	5.6	9.0	82	18	 **Ia,b,c**
	Ring B	5.7	7.1	50	50	
Ib[#]	Ring A	5.5	8.6	72	28	
	Ring B	5.5	6.5	36	64	
Ic[#]	Ring A	6.9	7.2	73	27	
	Ring B	5.6	6.8	44	56	

[#]The A- and B-ring protons were assigned based on 2D-COSY NMR experiments

Compound **Ic**: 2D-COSY ^{1}H NMR





Compound Ib: Temperature dependent ^{1}H-NMR shift in H-6 proton