

Supplementary Material

Synthesis, antimicrobial activity and molecular docking study of some novel cyclophanes with imino intra annular functionality

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Table S1 Antimicrobial activity of imino cyclophanes **1-7** by well diffusion assay

Imino Cyclophane	Concentration in $\mu\text{g/mL}$	Diameter of zone of inhibition in mm				
		<i>B. Subtilus</i>	<i>K. pneumonia</i>	<i>E. coli</i>	<i>S. aureus</i>	<i>C. albicans</i>
1	50	-	-	13	-	13
	75	-	-	14	13	14
	100	13	15	15	16	15
2	50	-	-	11	11	-
	75	12	13	12	13	-
	100	14	14	14	15	13
3a	50	12	-	-	13	-
	75	14	13	14	14	13
	100	16	16	17	17	16

	50	15	-	14	-	12
3b	75	17	12	18	-	14
	100	18	13	23	-	16
	50	-	13	-	-	13
3c	75	13	15	13	14	15
	100	15	17	14	18	17
	50	-	-	13	-	-
4a	75	-	-	14	-	13
	100	15	14	17	15	16
	50	-	-	15	-	-
4b	75	-	-	16	-	-
	100	14	17	17	-	16
	50	-	-	14	-	-
5	75	-	-	16	13	13
	100	-	15	18	15	14
	50	12	-	-	-	-
6	75	13	-	12	-	13
	100	16	14	16	14	16
	50	-	-	-	12	-
7	75	15	-	14	14	14
	100	16	-	17	17	18
	Vancomycin (1mg/mL)	22	22	24	20	NA
	Fluconazole (1mg/mL)	NA	NA	NA	NA	-
	Control	-	-	-	-	-

NA – not applicable; - – no inhibition

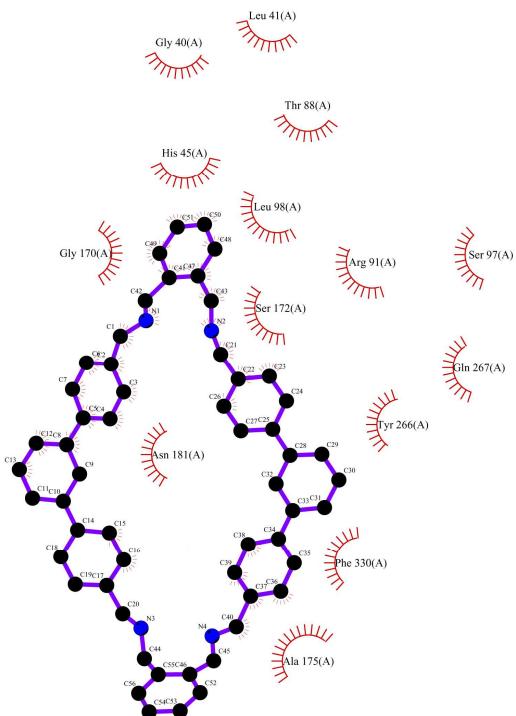


Figure S1. Ligplot results: Binding of ligand – imino cyclophane **3** on A-Chain amino acids of DNA gyrase B (PDB ID: 2Y3P) with 14 hydrophobic interactions.

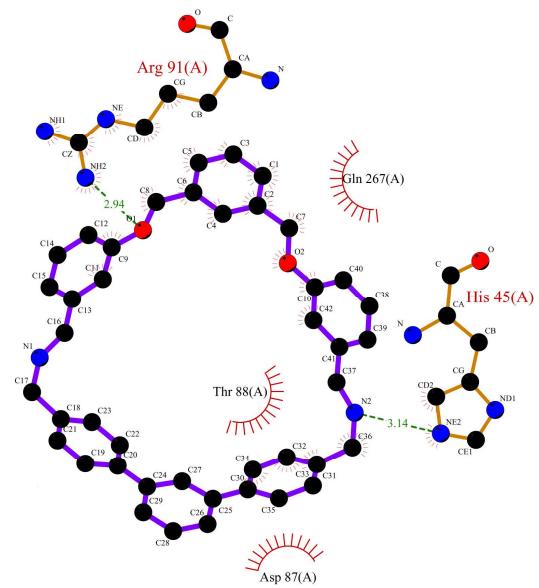


Figure S2. Ligplot results: Binding of ligand – imino cyclophane **4a** on A-Chain amino acids of DNA gyrase B (PDB ID: 2Y3P) with 2 hydrogen bonds and 3 hydrophobic interactions.

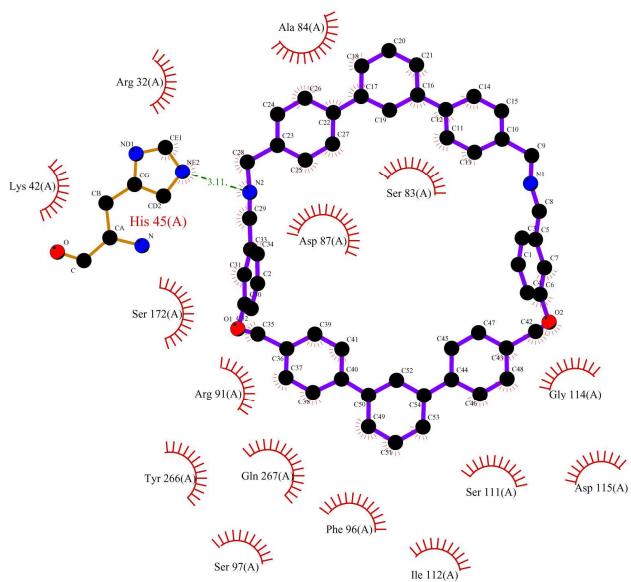
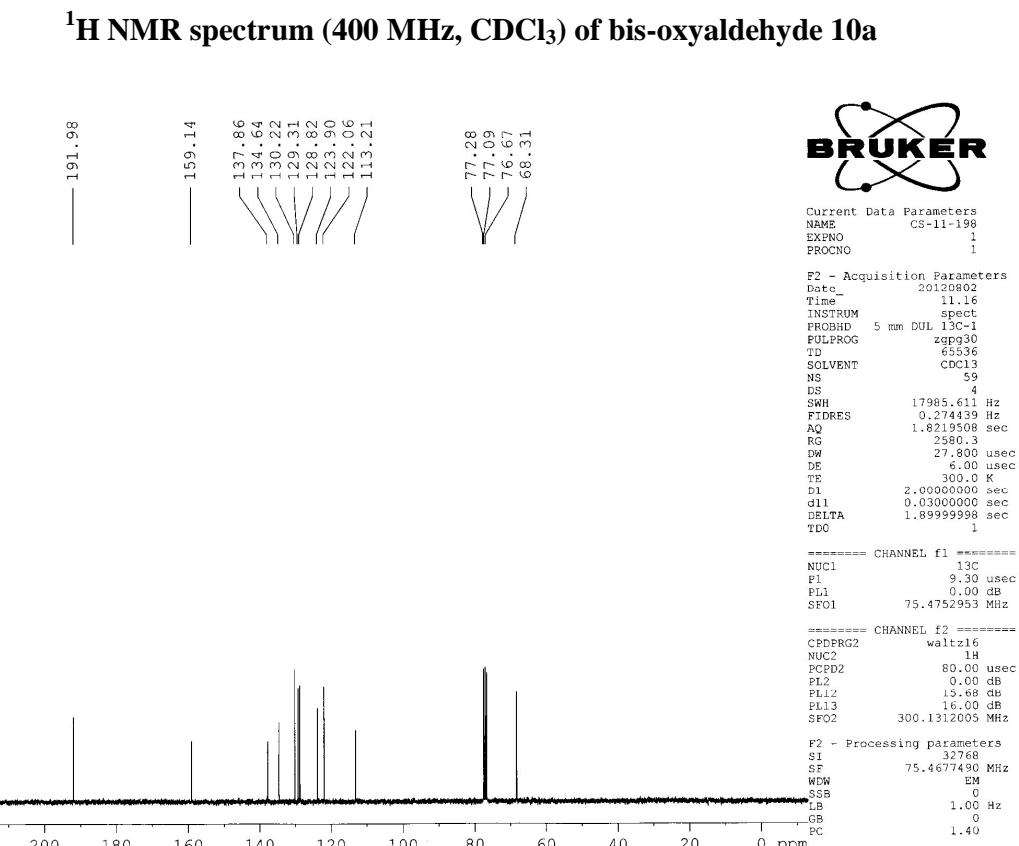
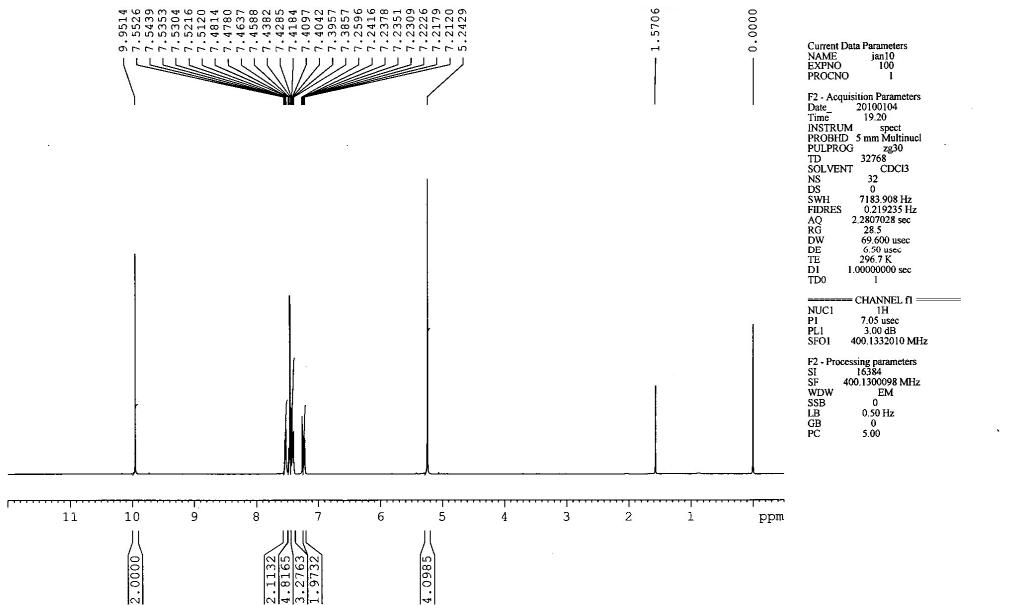
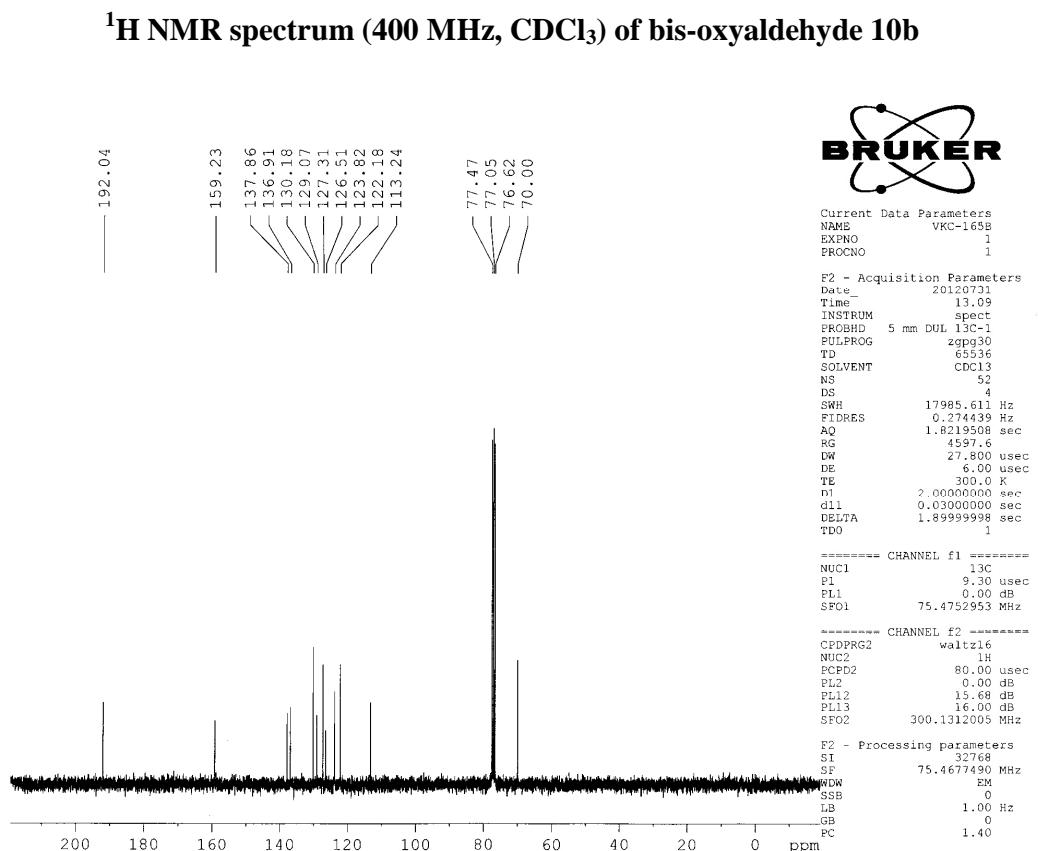
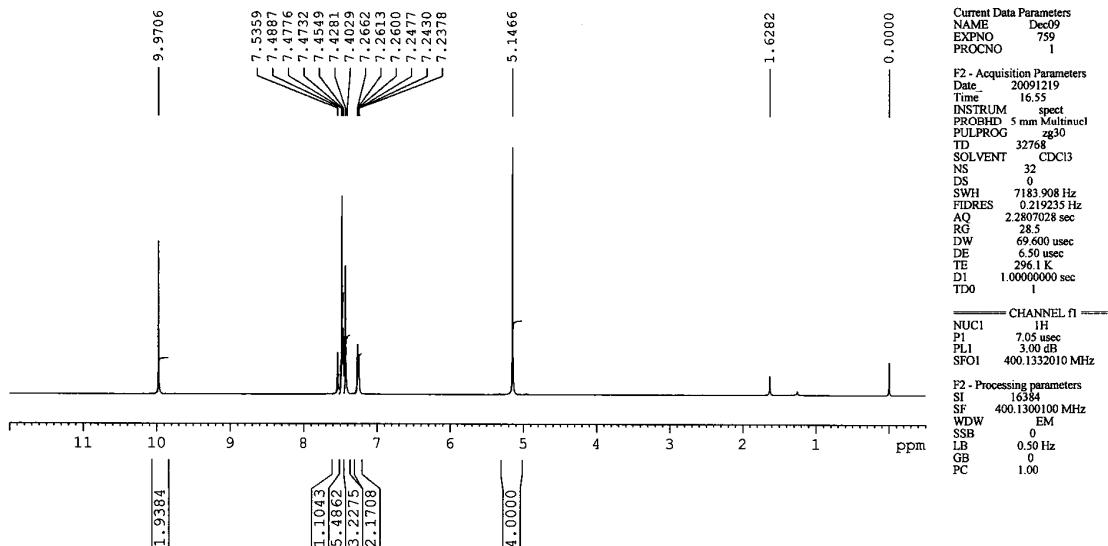
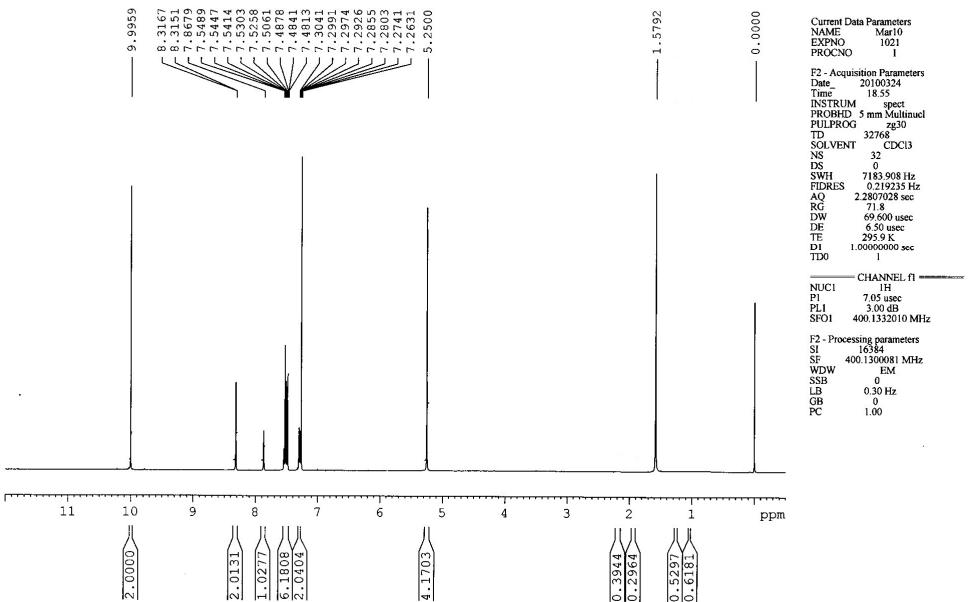
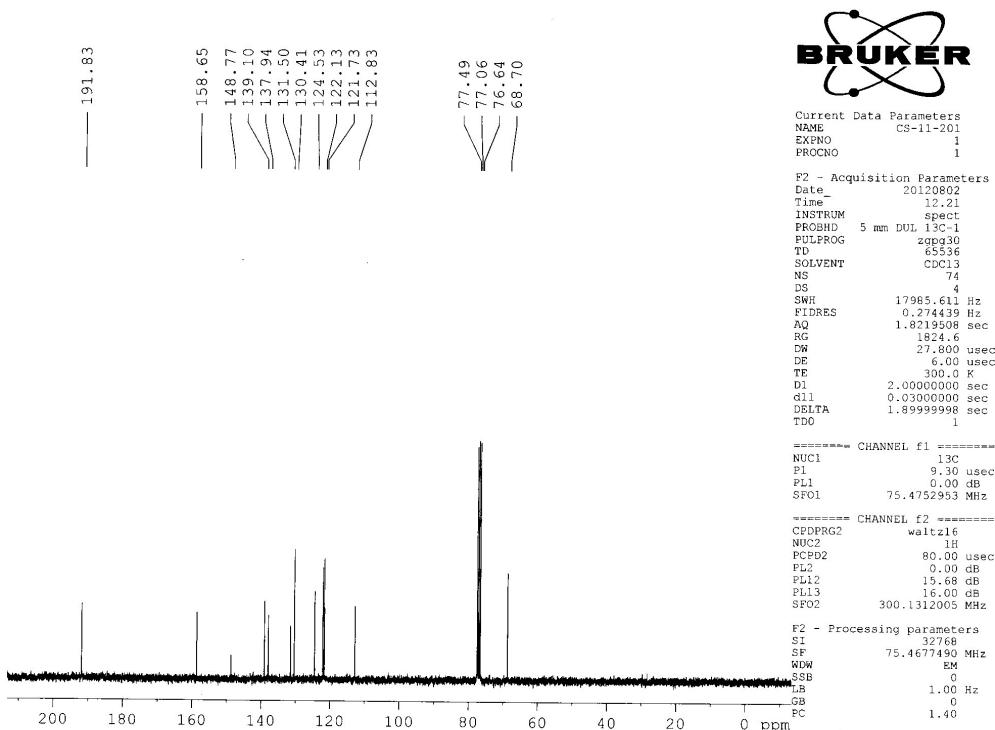
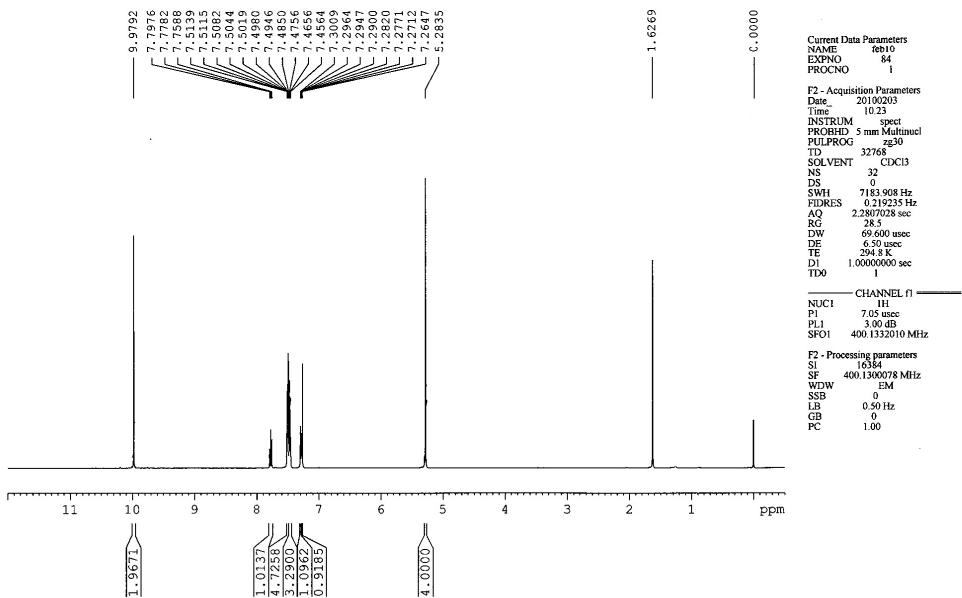


Figure S3. Ligplot results: Binding of ligand 999 (Z) – imino cyclophane **7** on A-Chain amino acids of DNA gyrase B (PDB ID: 2Y3P) with 1 hydrogen bond and 15 hydrophobic interactions.

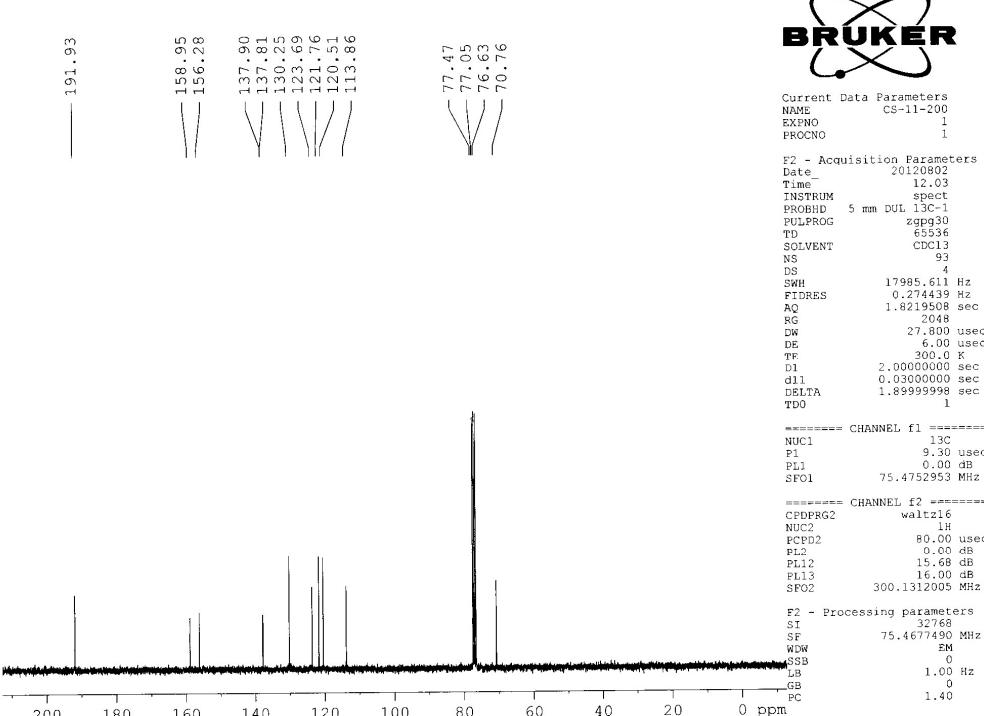
**1^H NMR spectrum (400 MHz, CDCl₃) of bis-oxyaldehyde 10a**

¹³C NMR spectrum (100 MHz, CDCl₃) of bis-oxyaldehyde 10b

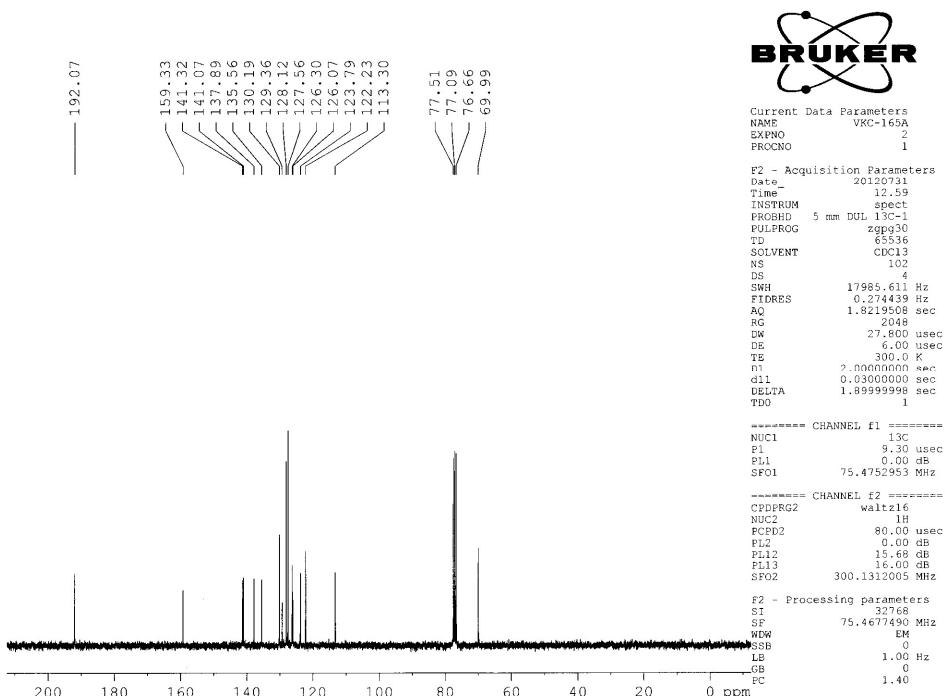
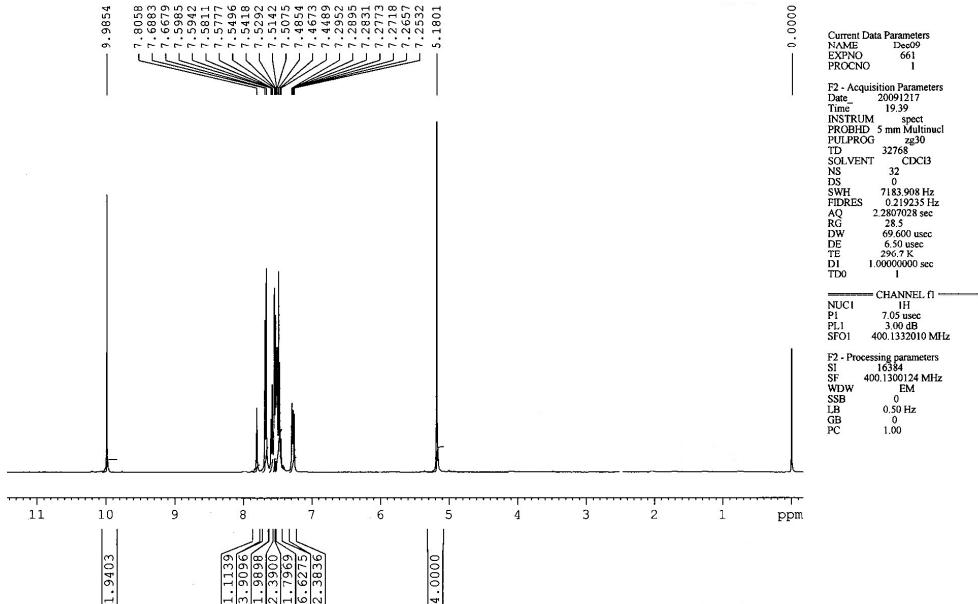
**¹H NMR spectrum (400 MHz, CDCl₃) of bis-oxyaldehyde 11****¹³C NMR spectrum (100 MHz, CDCl₃) of bis-oxyaldehyde 11**



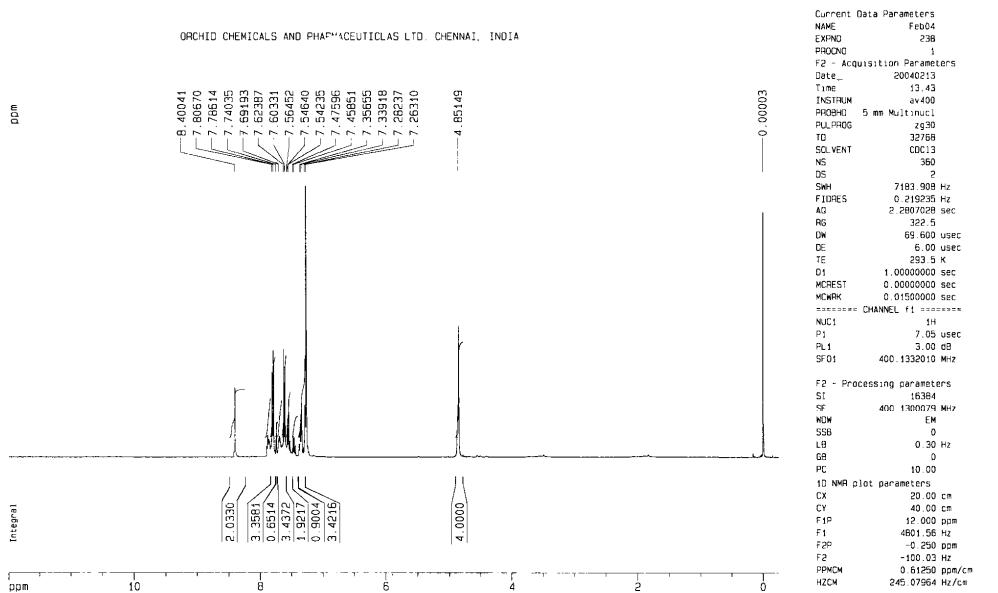
¹H NMR spectrum (400 MHz, CDCl₃) of bis-oxyaldehyde 12



¹³C NMR spectrum (100 MHz, CDCl₃) of bis-oxyaldehyde 12

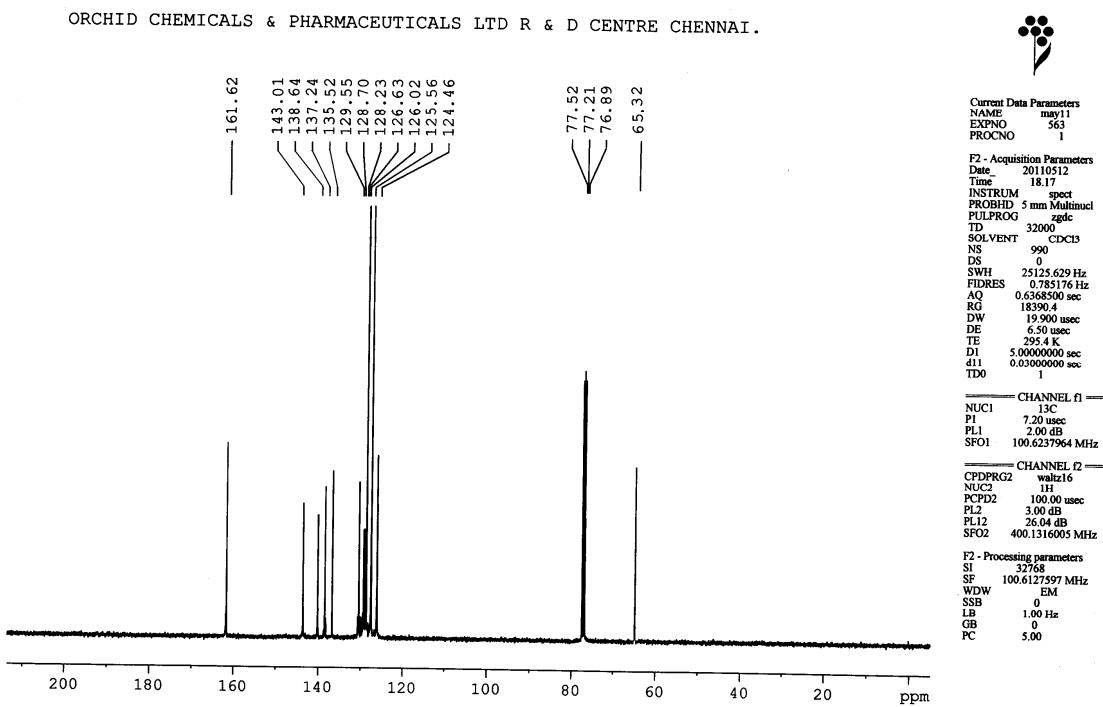


¹³C NMR spectrum (100 MHz, CDCl₃) of bis-oxyaldehyde 13

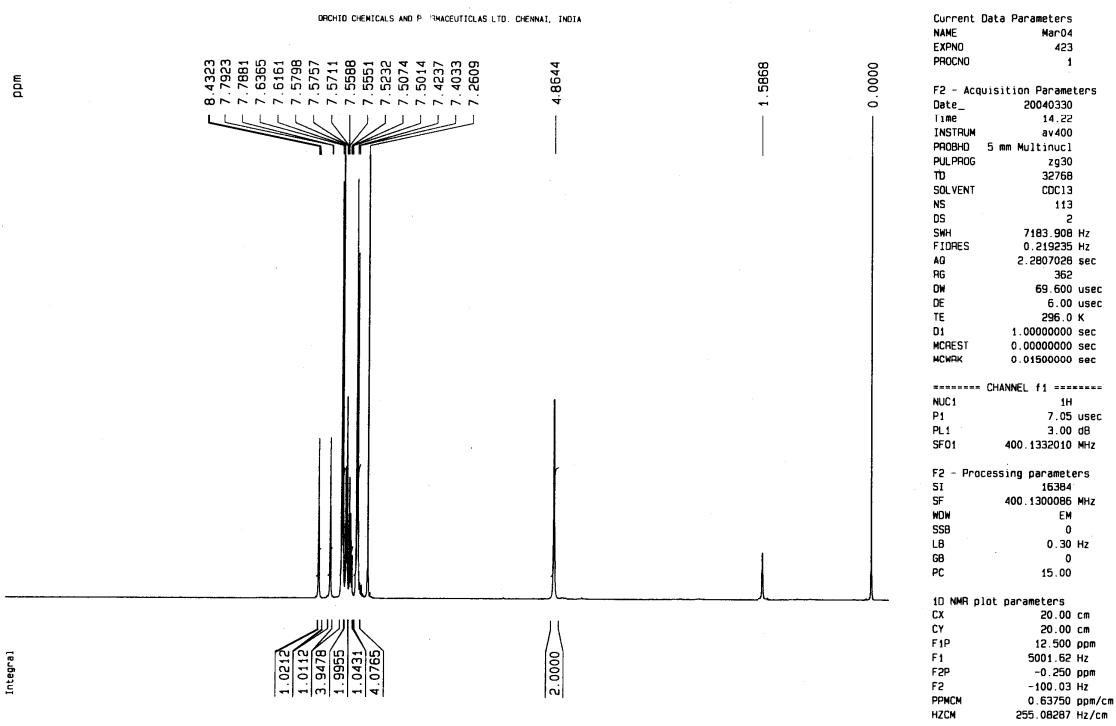


¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 1

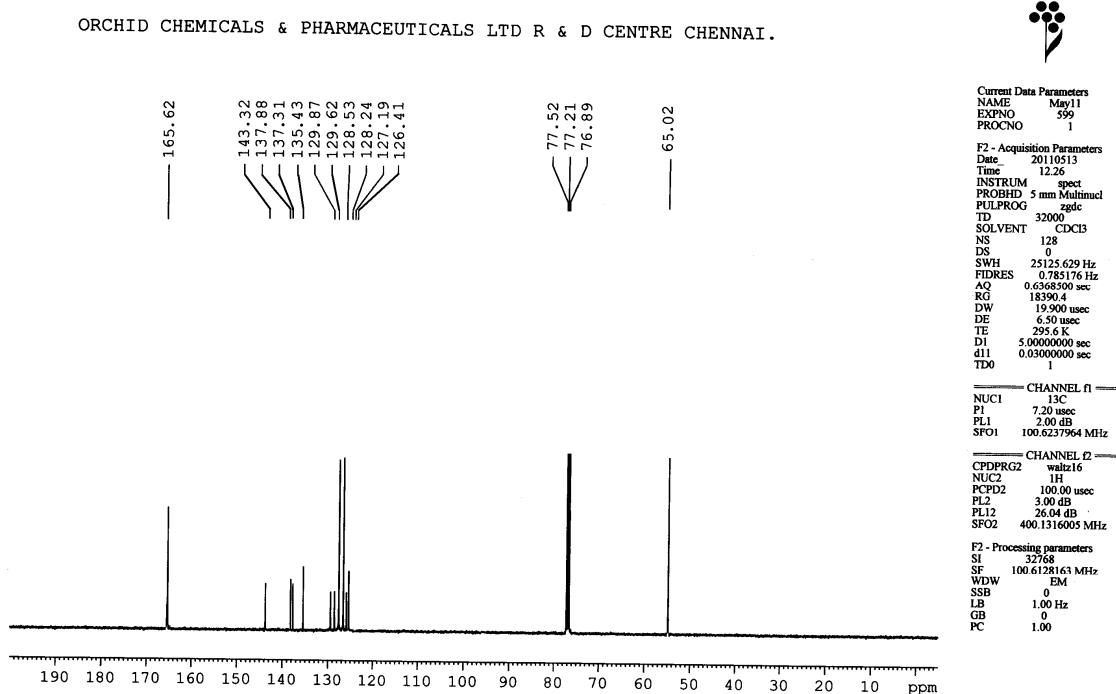
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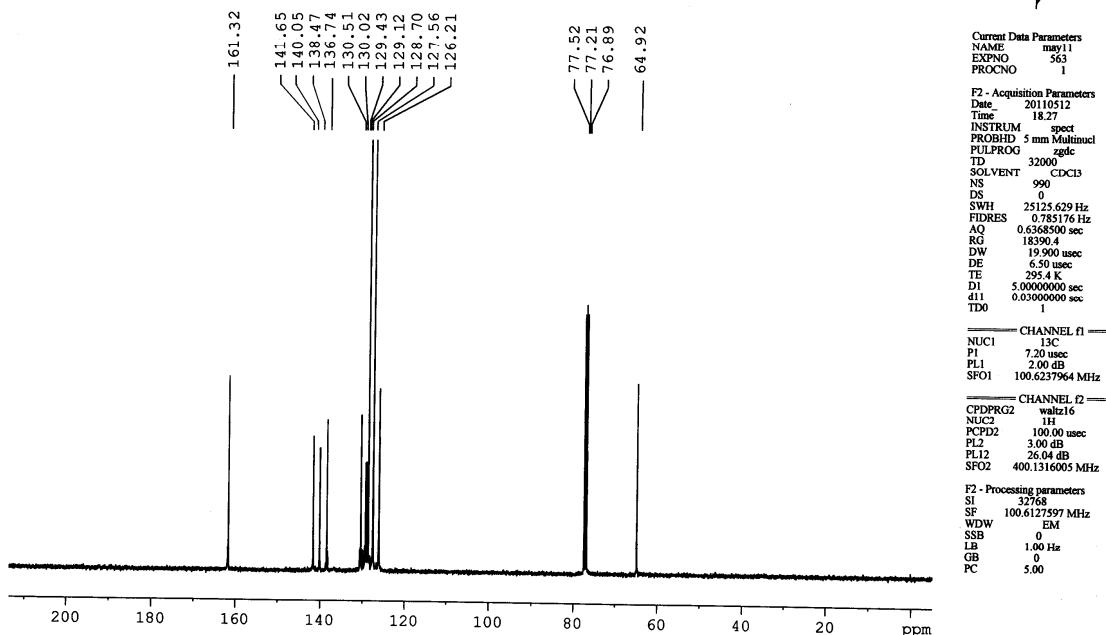
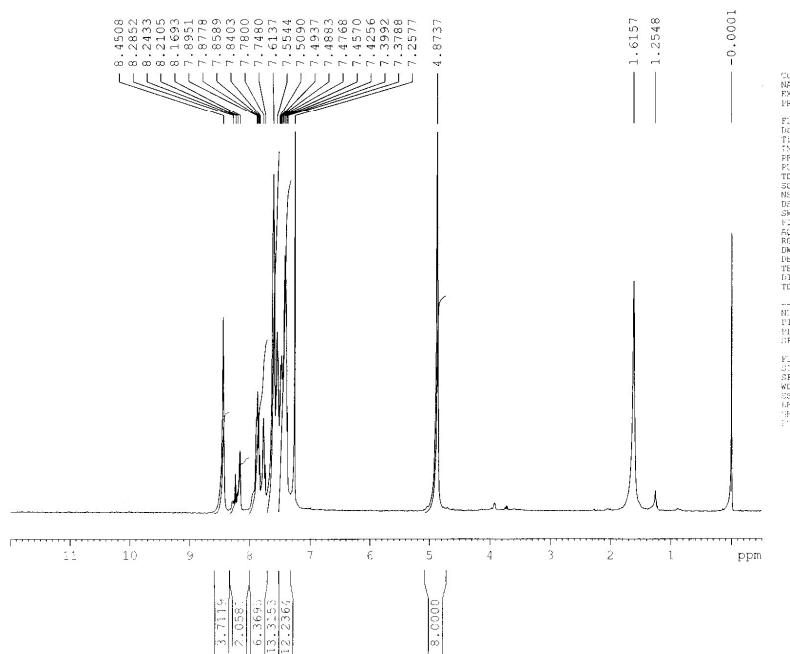
¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 1



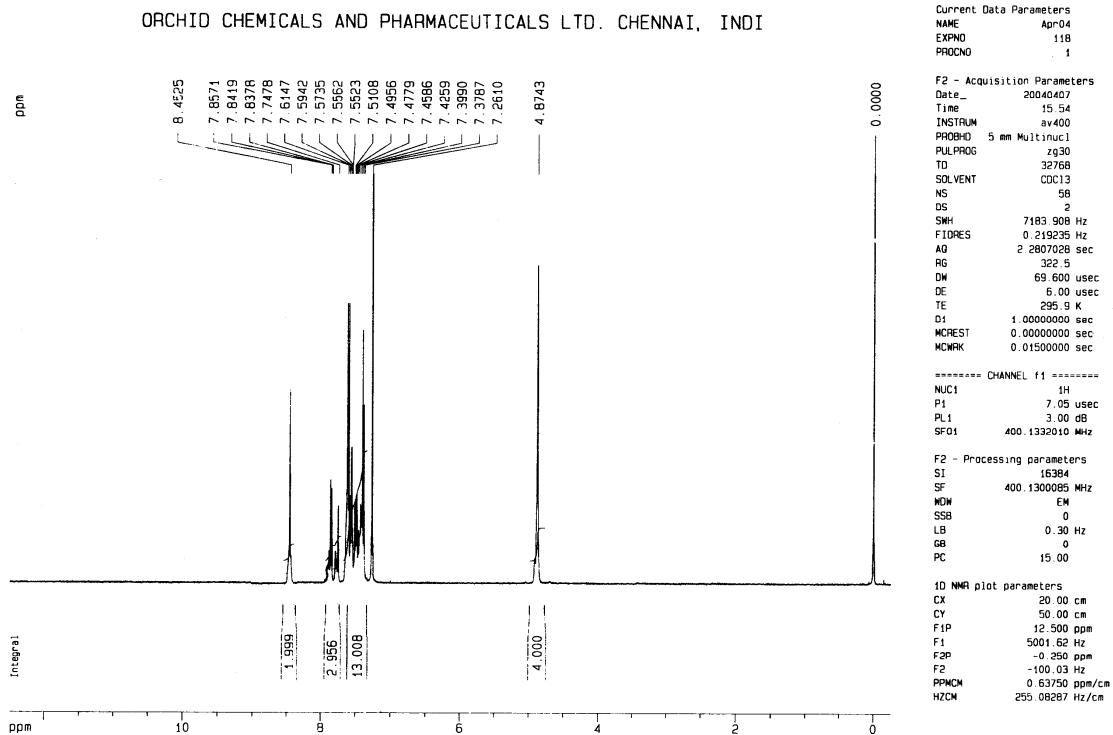
¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 2



¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 2

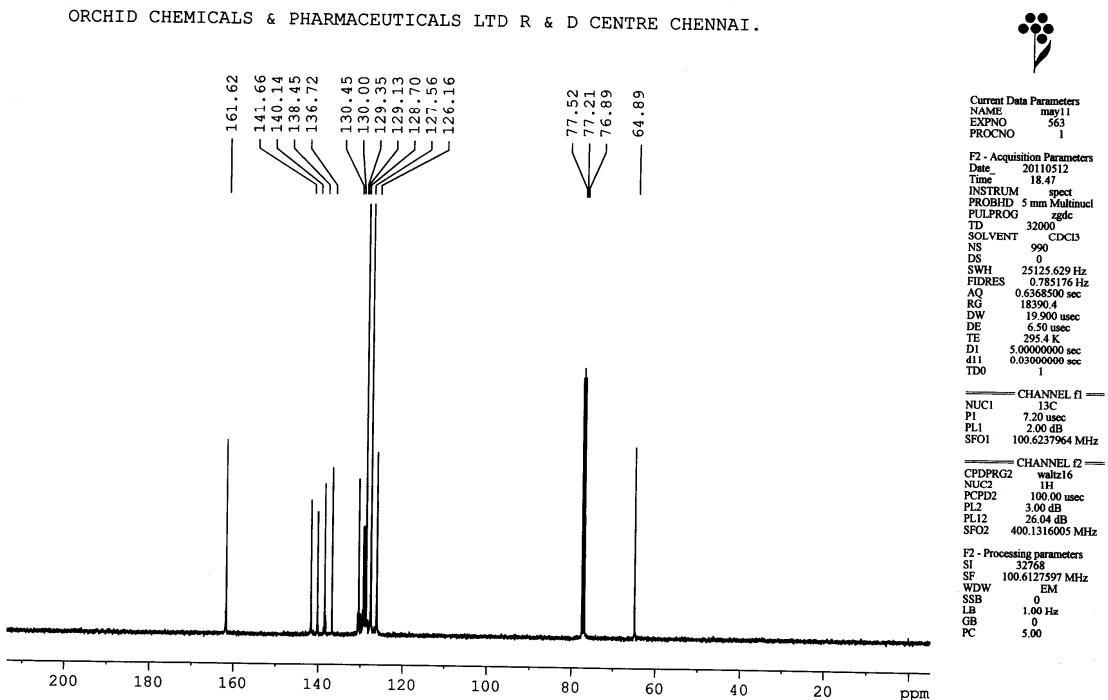


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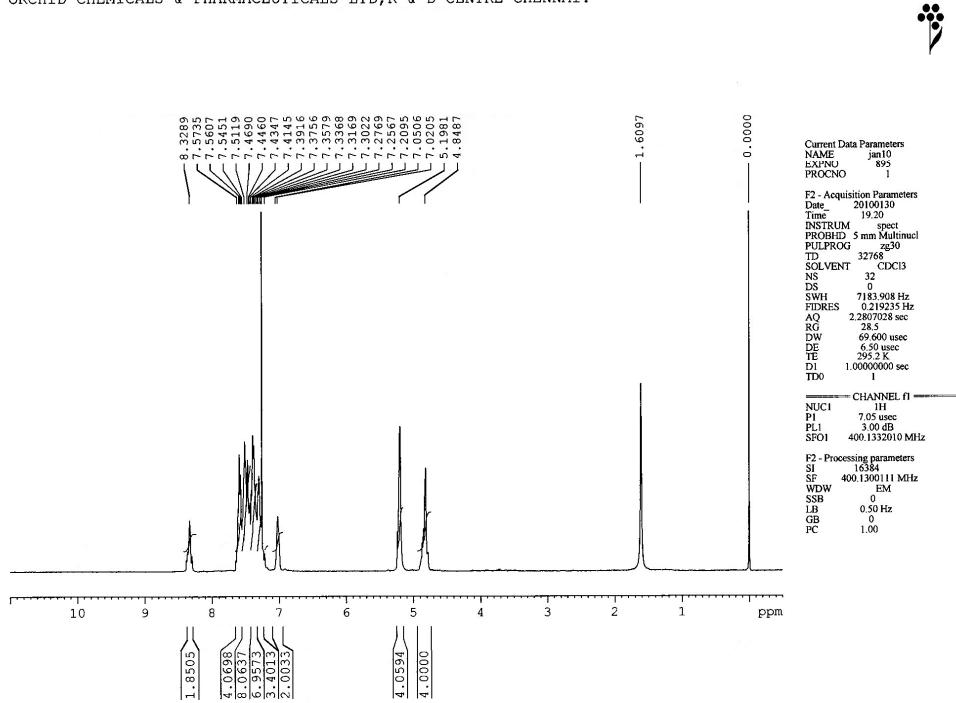
¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 3b

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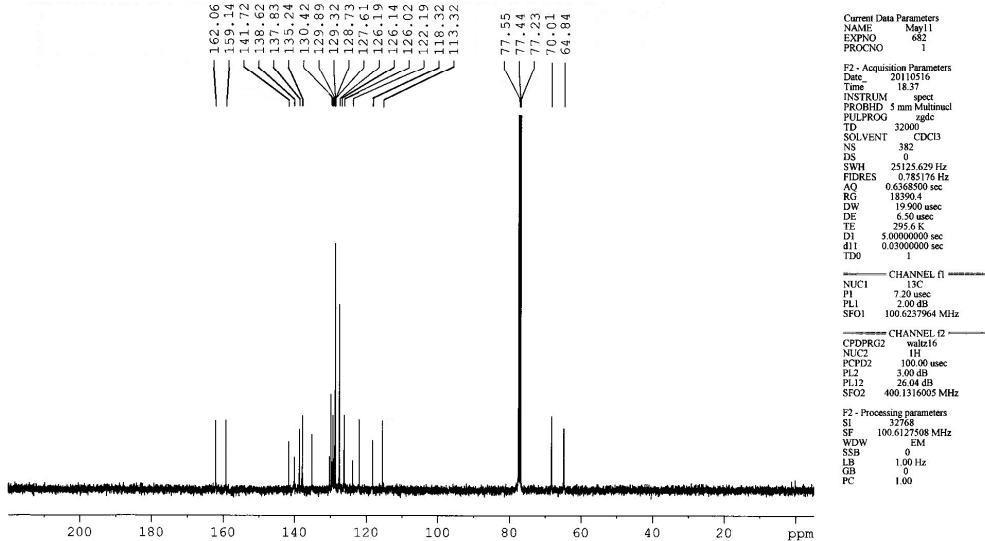
¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 3b

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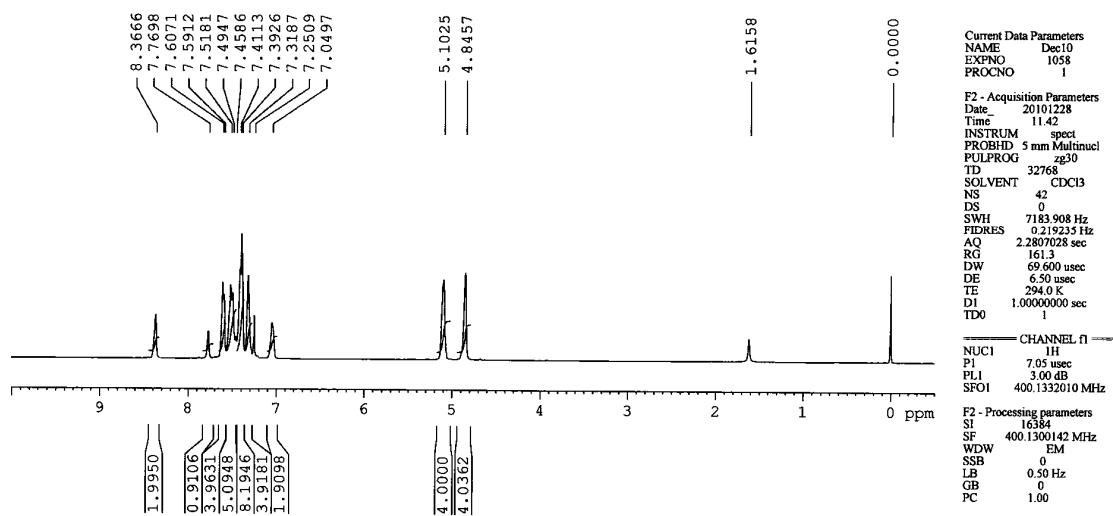
¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 4a

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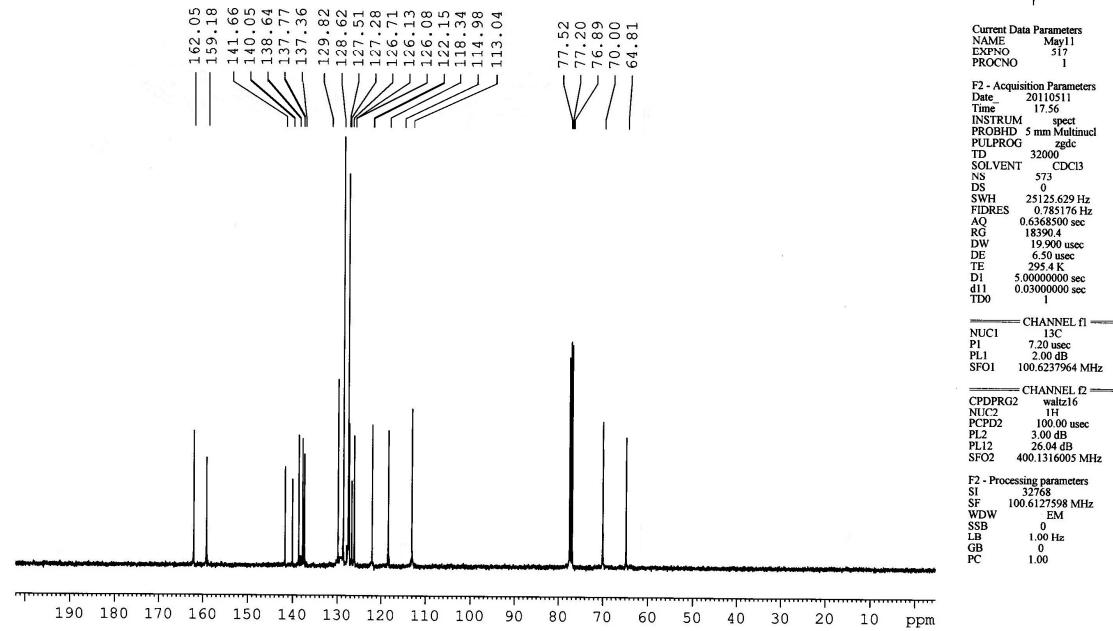
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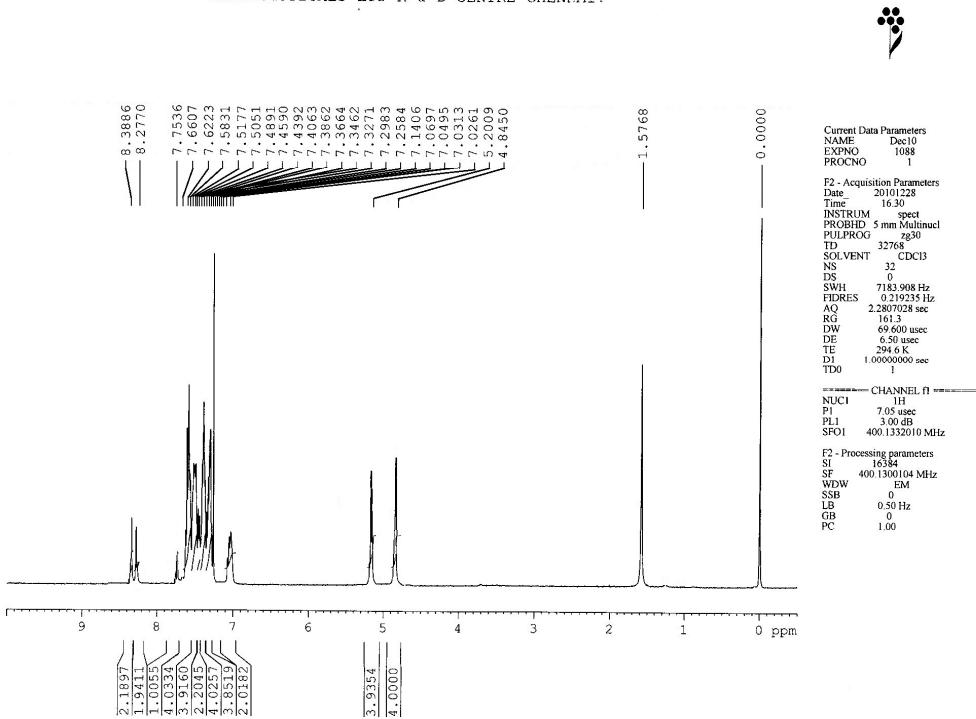
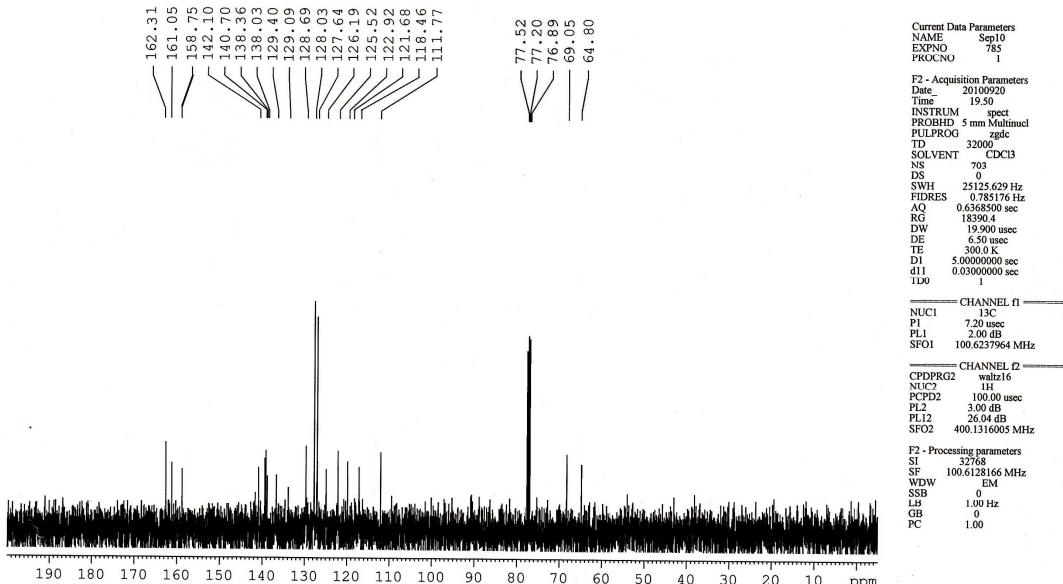


¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 4b

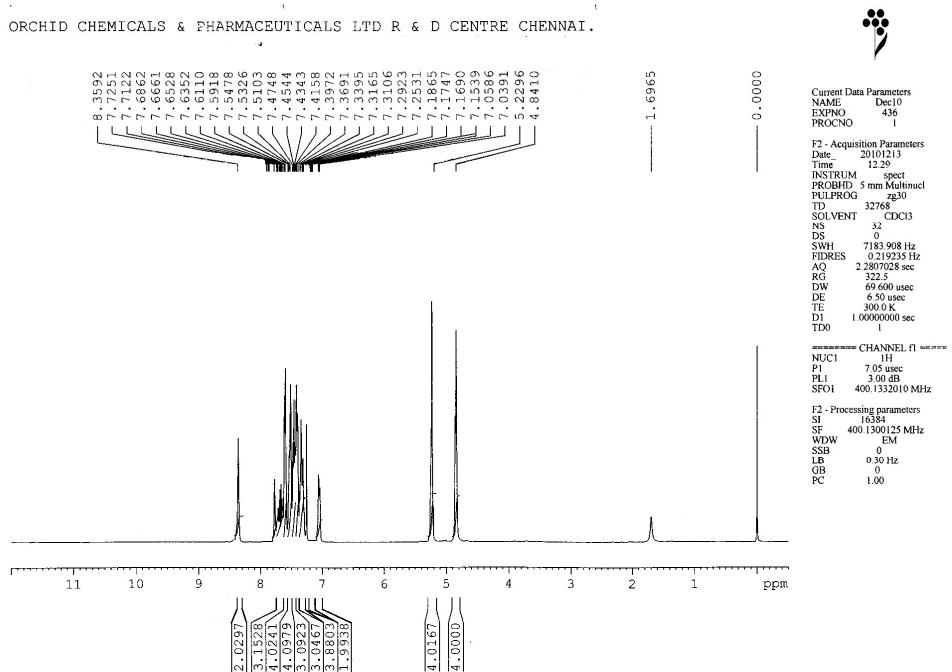
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¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 4a

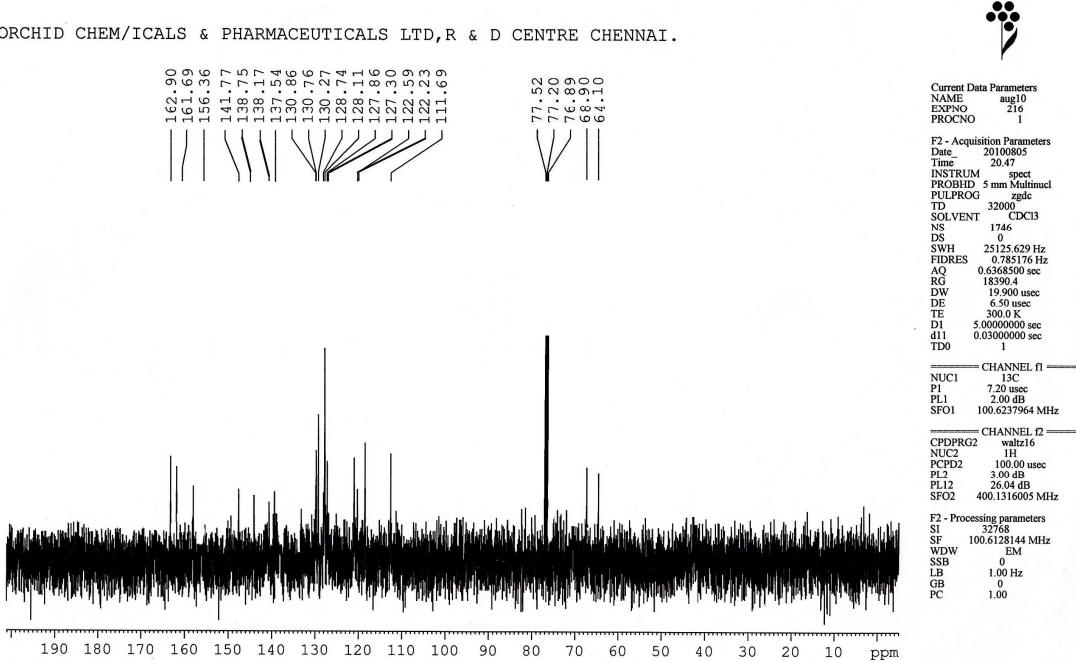
**¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 5****¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 5**

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¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 6

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¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 6

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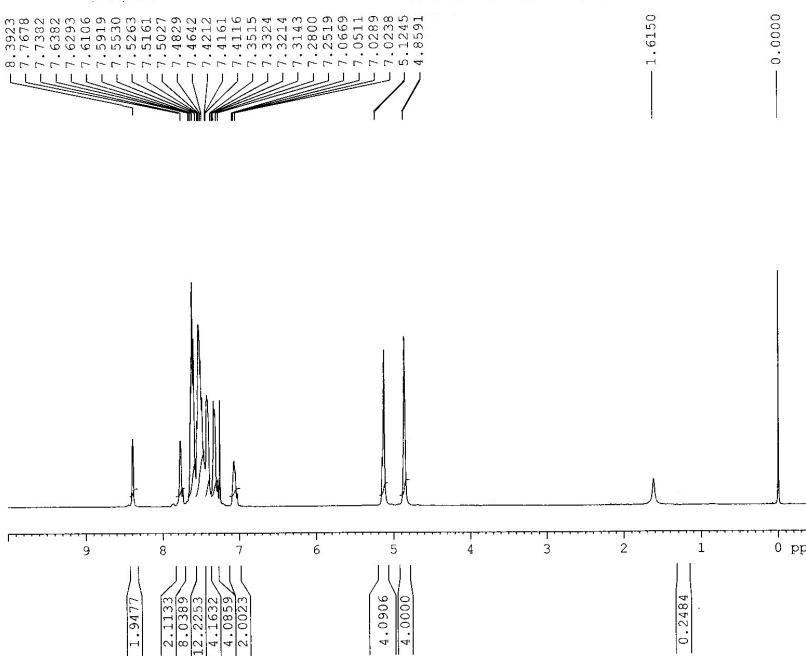


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¹H NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 7

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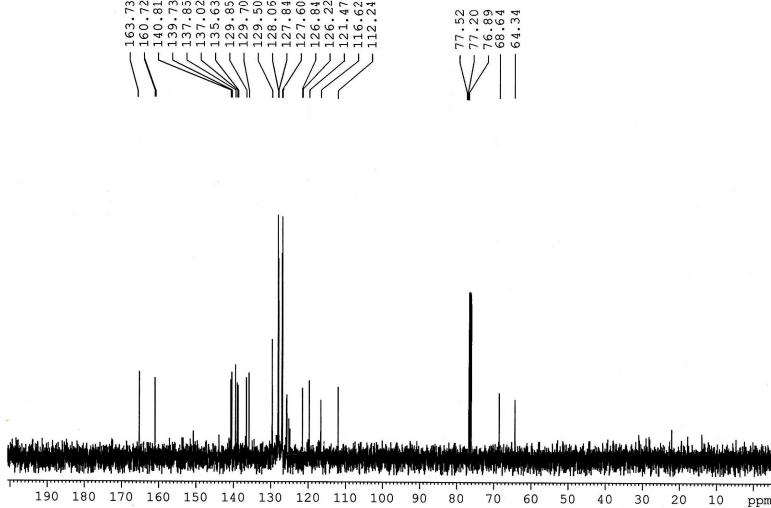
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¹³C NMR spectrum (400 MHz, CDCl₃) of imino cyclophane 7