

Figure S3. 2D COSY of compound **I** at ambient temperature in D₂O.

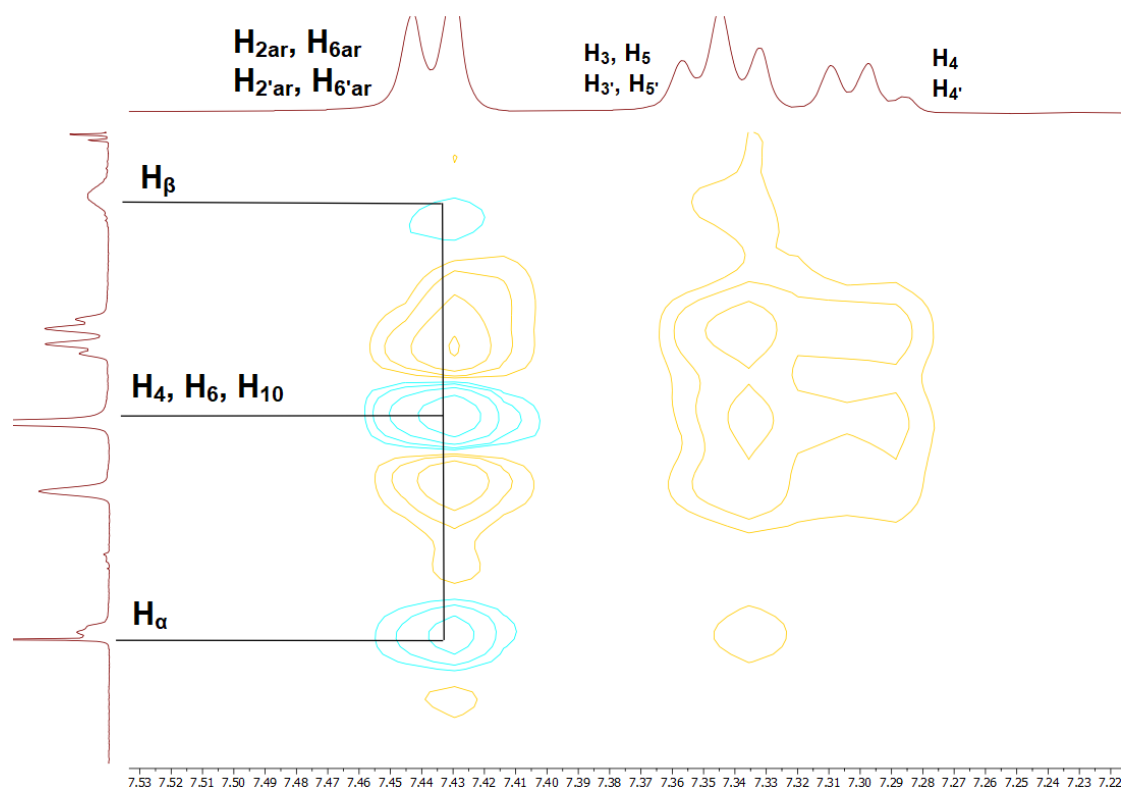


Figure S4. 2D NOESY of compound **I** at ambient temperature in D₂O.

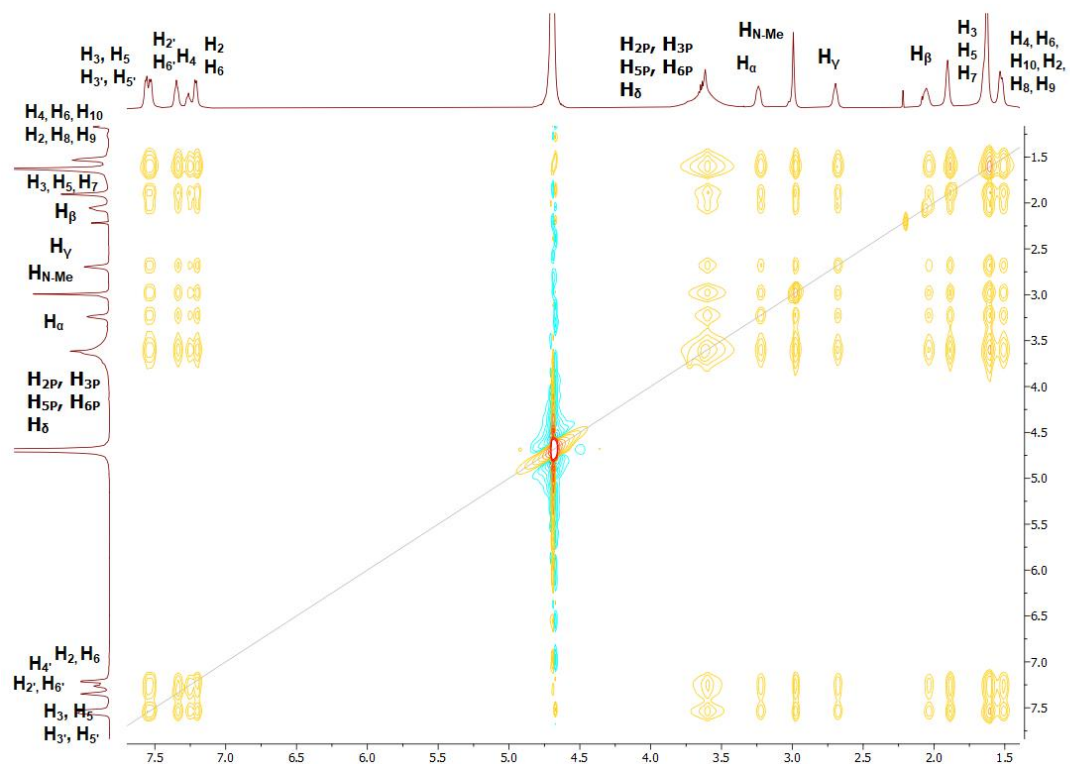


Figure S6: 2D NOESY of compound II at ambient temperature in D₂O.

Tables

Table S1. ¹H chemical structure shifts of compound **I** using a combination of 1D and 2D NMR experiments.

Position	¹ H	Multiplicity	2D NOESY	2D COSY
H_α	2.69	d.		H _β (1.30 ppm)
H_β	1.30	Br. S	H _{6ar} , H _{2ar} , H _{2'ar} , H _{6'ar}	
H_γ	2.21	Multiple	H _{6ar} , H _{2ar} , H _{2'ar} , H _{6'ar}	H _β (1.30 ppm)
H₂	1.59	d.d.		
H₃	1.91	s.		
H₄	1.77	s.	H _{6ar} , H _{2ar} , H _{2'ar} , H _{6'ar}	
H₅	1.91	s.		
H₆	1.77	s.	H _{6ar} , H _{2ar} , H _{2'ar} , H _{6'ar}	
H₇	1.91	s.		
H₈	1.59	d.d.		
H₉	1.59	d.d.		
H₁₀	1.77	s.	H _{6ar} , H _{2ar} , H _{2'ar} , H _{6'ar}	
H_{2ar}	7.43	d.		
H_{3ar}	7.34	t.		
H_{4ar}	7.29	t.		
H_{5ar}	7.34	t.		
H_{6ar}	7.43	d.		
H_{2'ar}	7.43	d.		
H_{3'ar}	7.34	t.		
H_{4'ar}	7.29	t.		
H_{5'ar}	7.34	t.		
H_{6'ar}	7.43	d.		
H_{2p}	3.07	very br. s.		
H_{3p}	3.07	very br. s.		
H_{5p}	3.07	very br. s.		
H_{6p}	3.07	very br. s.		
H_{N-Me}	2.69	d.		H _β (1.30 ppm)

Table S2. ^1H NMR chemical shifts of compound **II** derived from a combination of 1D and 2D homonuclear NMR experiments.

Position	^1H	Multiplicity	2D ^1H - ^1H NOESY	2D ^1H - ^1H COSY
H_a	2.70 ppm	s.	H_β $\text{H}_3, \text{H}_5, \text{H}_7$ $\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_{2\text{eq}}, \text{H}_{8\text{eq}}, \text{H}_{9\text{eq}}$	H_β (2.05)
H_β	2.05 ppm	d.	$\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
H_γ	3.21 ppm	d.	$\text{H}_{\text{N-Me}}$ H_a H_β $\text{H}_3, \text{H}_5, \text{H}_7$ $\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	H_β (2.05)
H_δ	3.61 ppm	br. multiplet		-
H_2	1.62 (eq) ppm 1.53 (ax) ppm	d.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
H_3	1.86 ppm	s.	$\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
H_4	1.53 ppm	s.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
H_5	1.86 ppm	s.	$\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
H_6	1.53 ppm	s.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
H_7	1.86 ppm	s.	$\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
H_8	1.62 (eq) ppm 1.53 (ax) ppm	d.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
H_9	1.62 (eq) ppm 1.53 (ax) ppm	d.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
H_{10}	1.53 ppm	s.	$\text{H}_3, \text{H}_5, \text{H}_7$	-
$\text{H}_{2\text{ar}}$	7.22 ppm	d.		-
$\text{H}_{3\text{ar}}$	~7.54 ppm	t.	$\text{H}_{\text{ar}2'}, \text{H}_{\text{ar}6'}$ $\text{H}_{4\text{ar}'}$ $\text{H}_{2\text{ar}}, \text{H}_{6\text{ar}}$ $\text{H}_3, \text{H}_5, \text{H}_7$ $\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
$\text{H}_{5\text{ar}}$	~7.54 ppm	t.	$\text{H}_{2'\text{ar}}, \text{H}_{6'\text{ar}}$ $\text{H}_{4\text{ar}'}$ $\text{H}_{2\text{ar}}, \text{H}_{6\text{ar}}$ $\text{H}_3, \text{H}_5, \text{H}_7$ $\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
$\text{H}_{6\text{ar}}$	7.22 ppm	d.		-
$\text{H}_{2'\text{ar}}$	7.34 ppm	d.		-
$\text{H}_{3'\text{ar}}$	~7.54 ppm	t.	$\text{H}_{\text{ar}2'}, \text{H}_{\text{ar}6'}$ $\text{H}_{4\text{ar}'}$ $\text{H}_{2\text{ar}}, \text{H}_{6\text{ar}}$ $\text{H}_3, \text{H}_5, \text{H}_7$ $\text{H}_4, \text{H}_6, \text{H}_{10}$ $\text{H}_2, \text{H}_8, \text{H}_9$	-
$\text{H}_{4'\text{ar}}$	7.26 ppm	t.		-
$\text{H}_{5'\text{ar}}$	~7.54 ppm	t.	$\text{H}_{2'\text{ar}}, \text{H}_{6'\text{ar}}$ $\text{H}_{4'\text{ar}}$ $\text{H}_{2\text{ar}}, \text{H}_{6\text{ar}}$	-

			H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉	
H _{6'ar}	7.34 ppm	d.		-
			H _α H _{N-Me} H _γ H _β H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{3ar} , H _{5ar} , H _{3'ar} , H _{5'ar} H _{2ar} , H _{6ar} H _{4ar}	
H _{2p}	3.61 ppm	br. multiplet		-
			H _α H _{N-Me} H _γ H _β H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{3ar} , H _{5ar} , H _{ar3'} , H _{5'ar} H _{2ar} , H _{6ar} H _{ar4}	
H _{3p}	3.61 ppm	br. multiplet		-
			H _α H _{N-Me} H _γ H _β H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{3ar} , H _{5ar} , H _{3'ar} , H _{5'ar} H _{2ar} , H _{6ar} H _{4ar}	
H _{5p}	3.61 ppm	br. multiplet		-
			H _α H _{N-Me} H _γ H _β H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{3ar} , H _{5ar} , H _{3'ar} , H _{5'ar} H _{2ar} , H _{6ar} H _{4ar}	
			H _α H _{N-Me} H _γ H _β H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{ar3} , H _{ar5} , H _{ar3'} , H _{ar5'} H _{ar2} , H _{ar6} H _{ar4}	
H _{6p}	3.61 ppm	br. multiplet		-
			H _α H _β H _γ H ₃ , H ₅ , H ₇ H ₄ , H ₆ , H ₁₀ H ₂ , H ₈ , H ₉ H _{2ar} , H _{6ar} H _{3ar} , H _{5ar} H _{3'ar} , H _{5'ar}	
H _{N-Me}	2.99 ppm	d.		-