

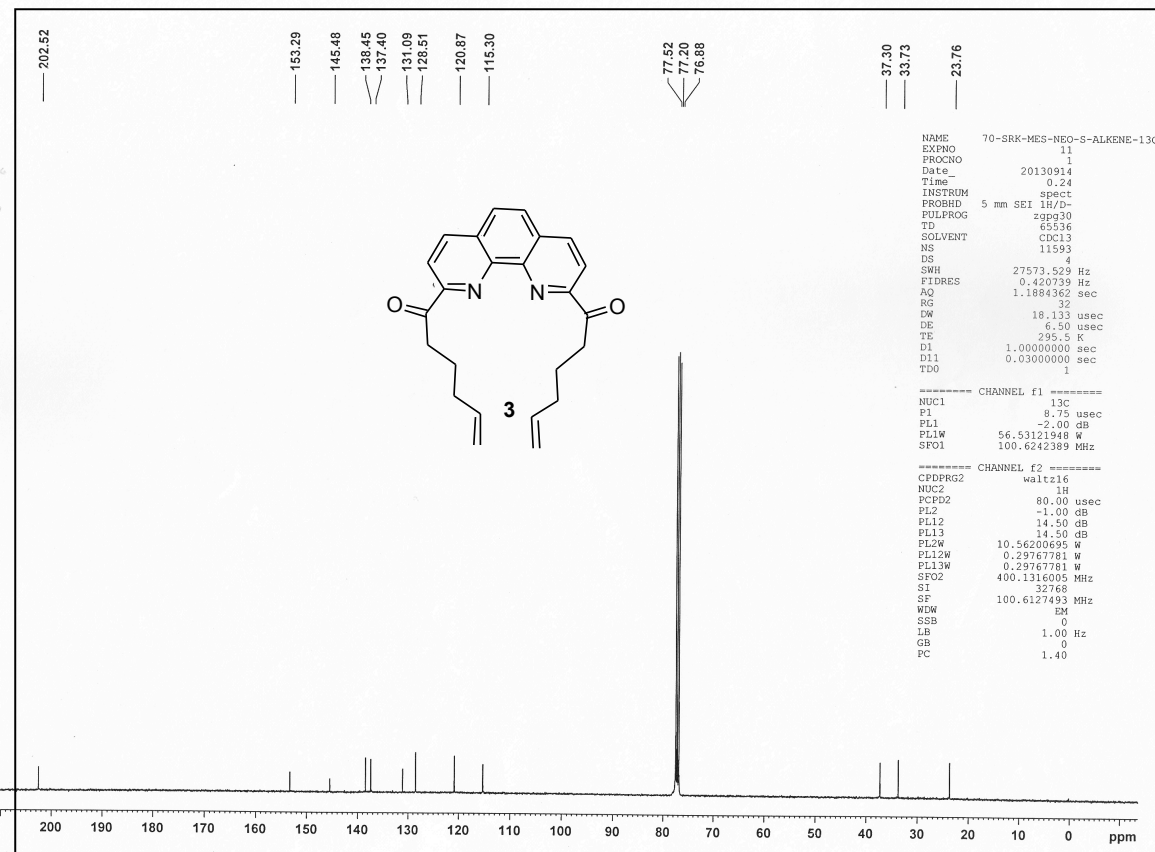
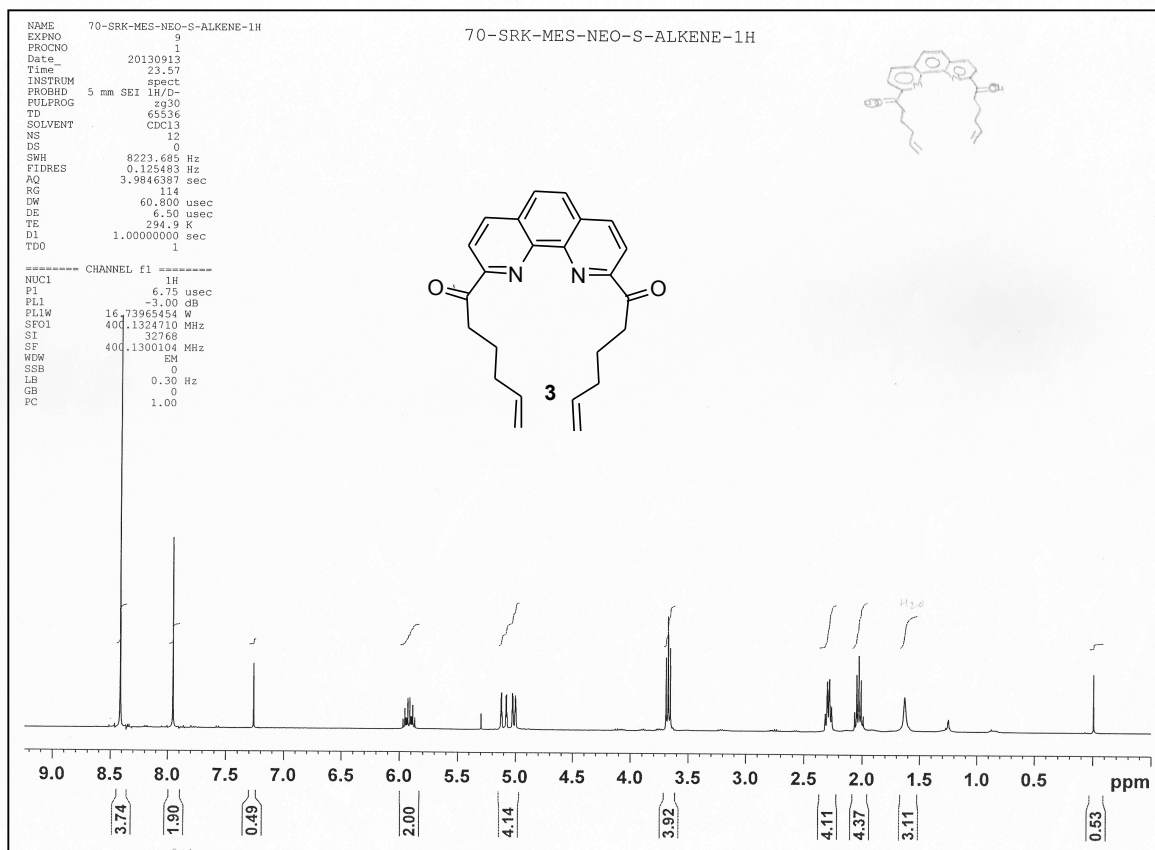
Synthesis of Phenanthroline based cyclophane derivatives via ring-closing metathesis as key step

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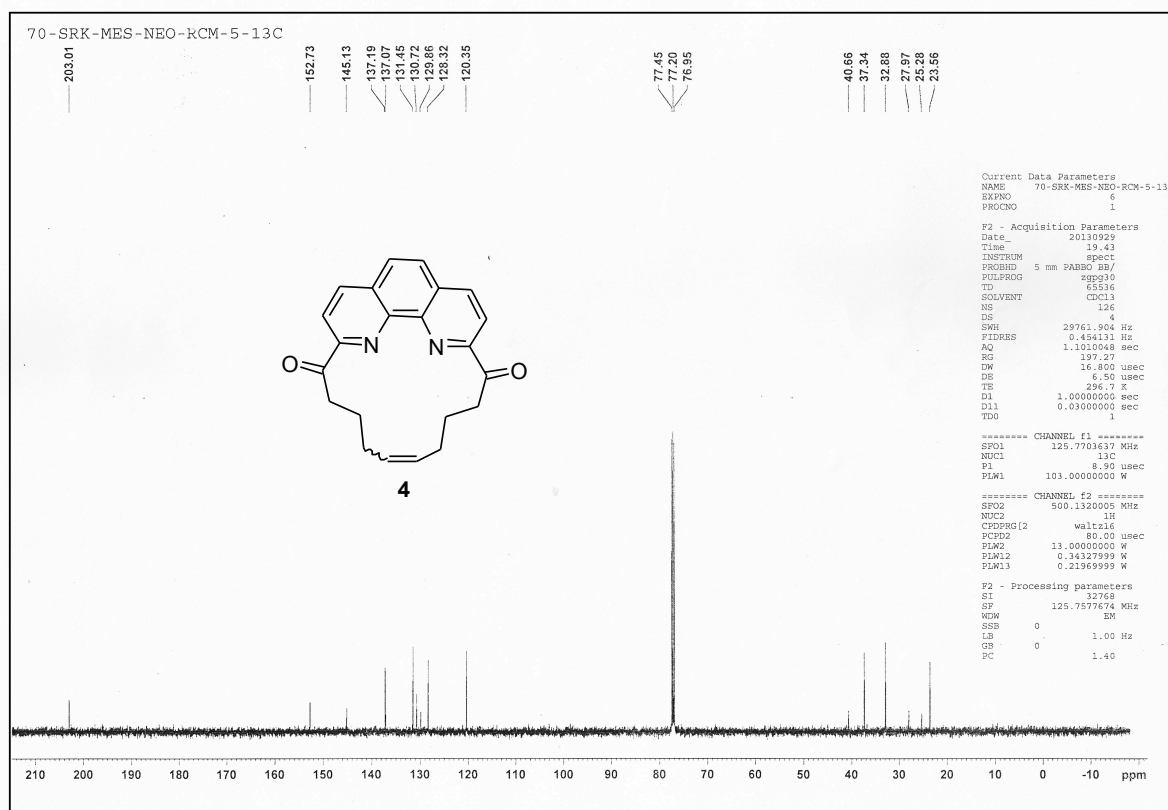
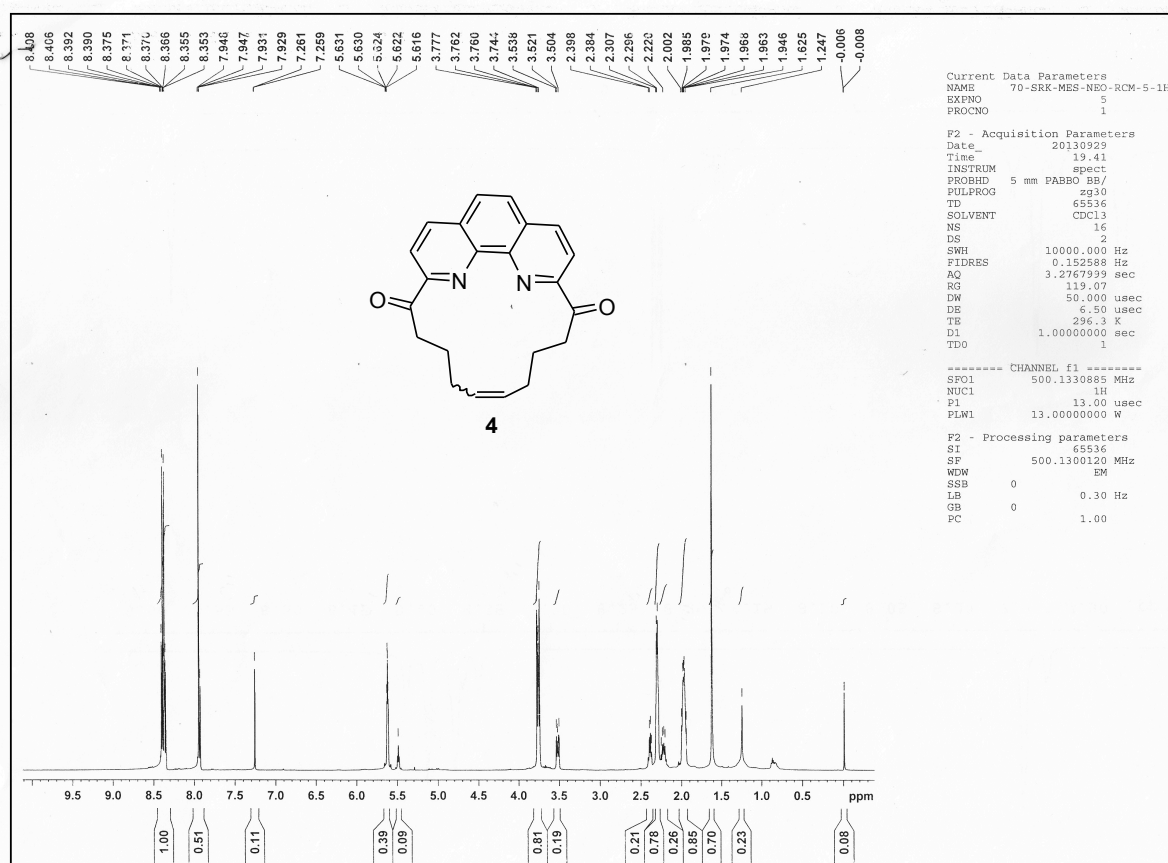
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1. ¹ H and ¹³ C NMR of compound 3	S2
2. ¹ H and ¹³ C NMR of compound 4	S3
3. ¹ H and ¹³ C NMR of compound 5	S4
4. ¹ H and ¹³ C NMR of compound 6a	S5
5. ¹ H and ¹³ C NMR of compound 6b	S6
17. X-ray crystallographic data and refinement parameters for 6a	S7
18. X-ray crystallographic data and refinement parameters for 6b	S8

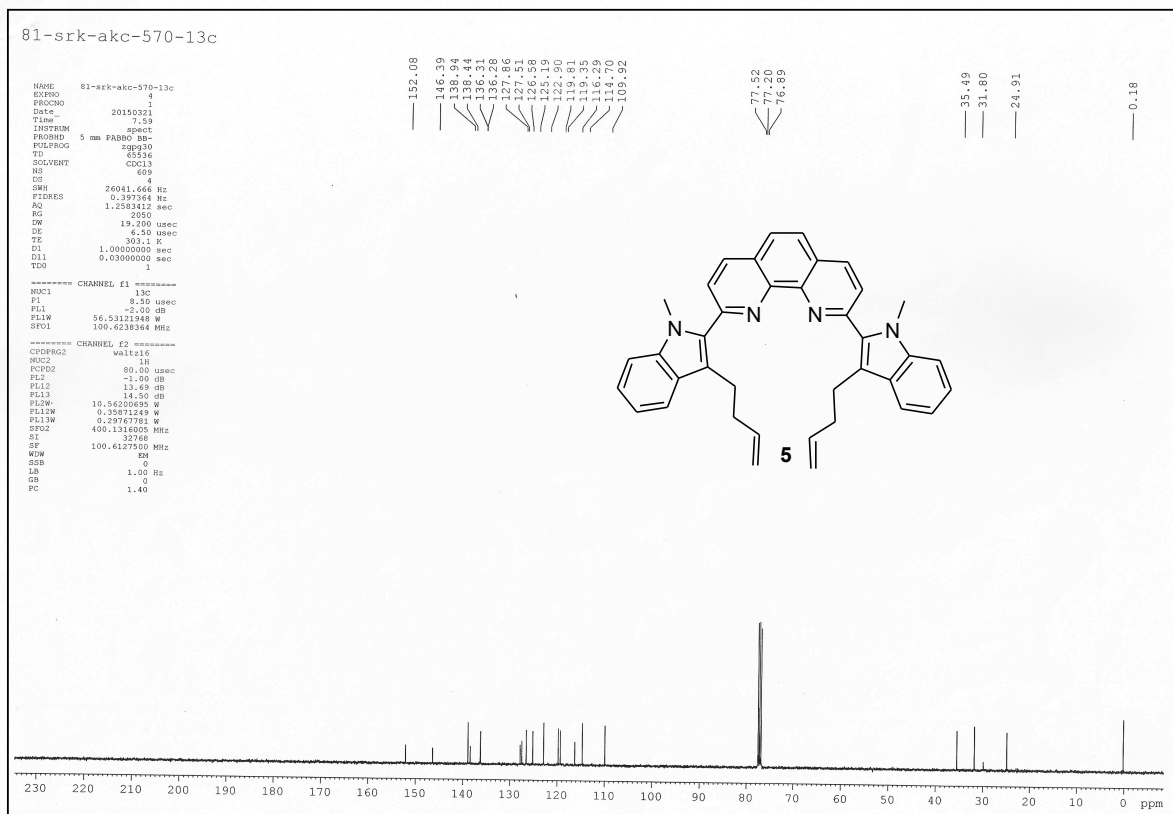
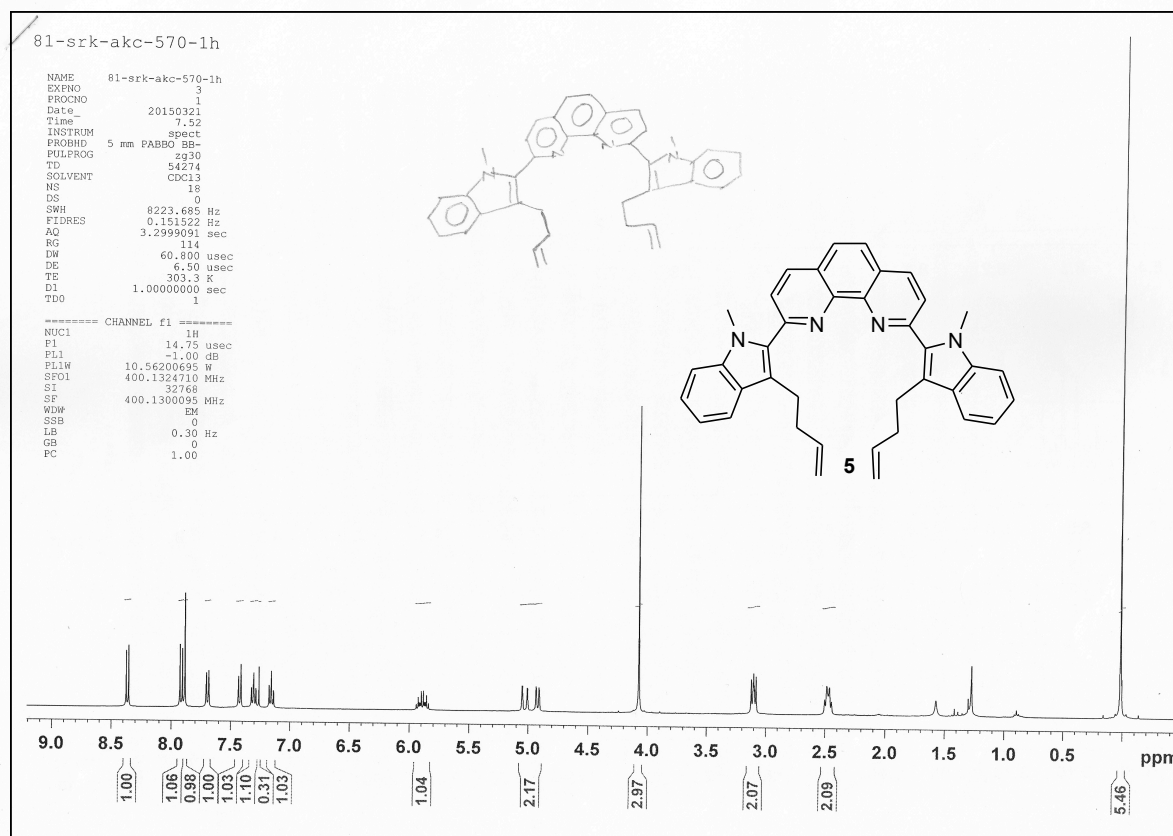
1H and 13C NMR of compound 3



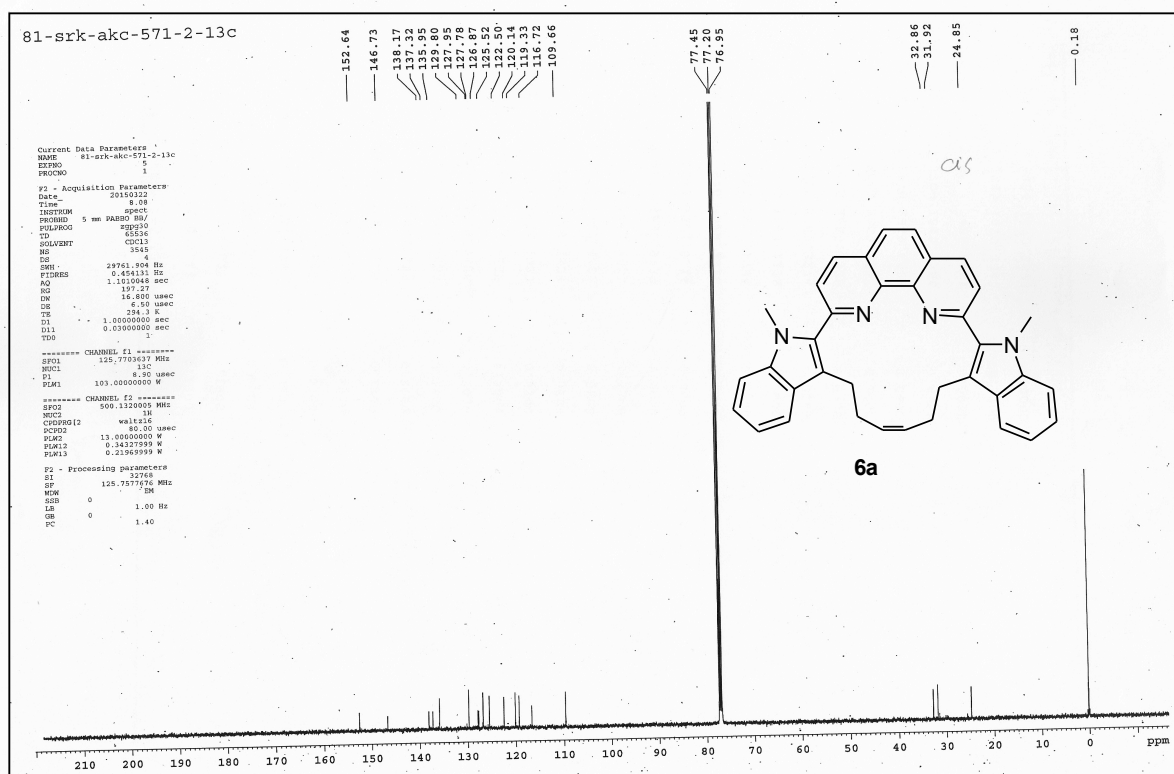
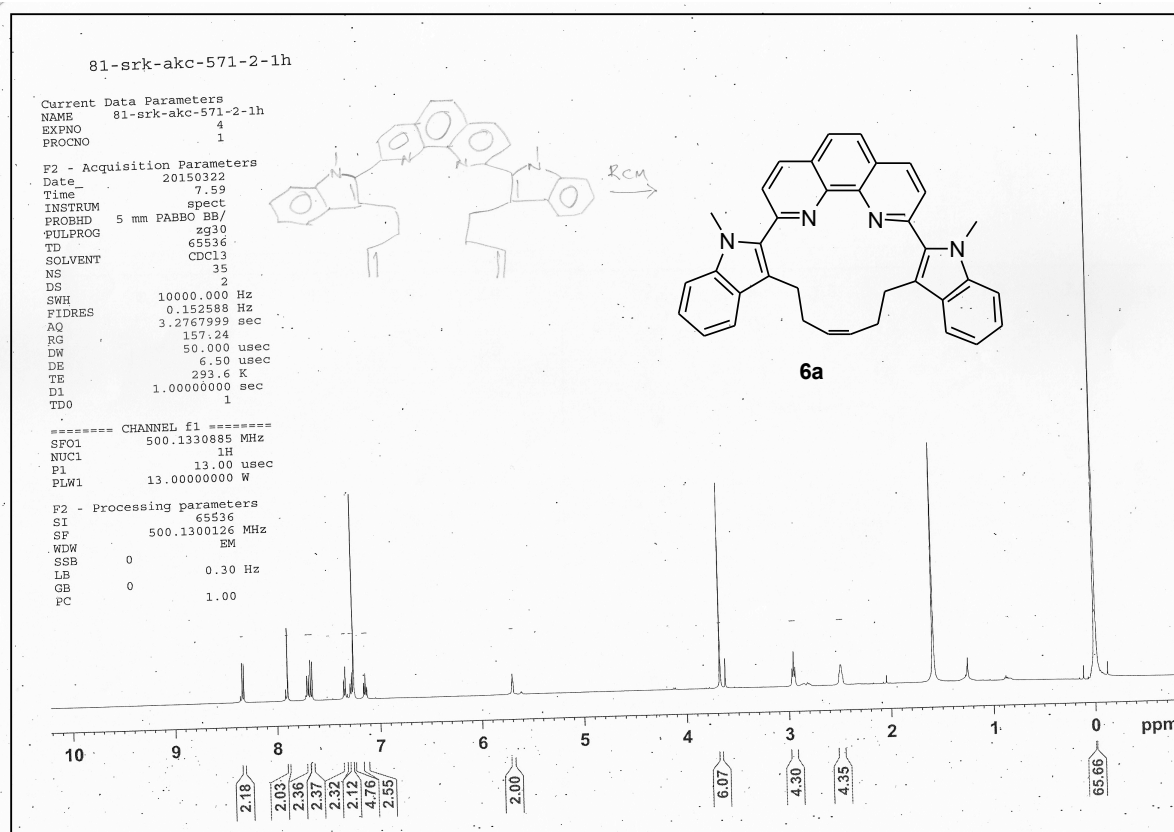
1H and 13C NMR of compound 4



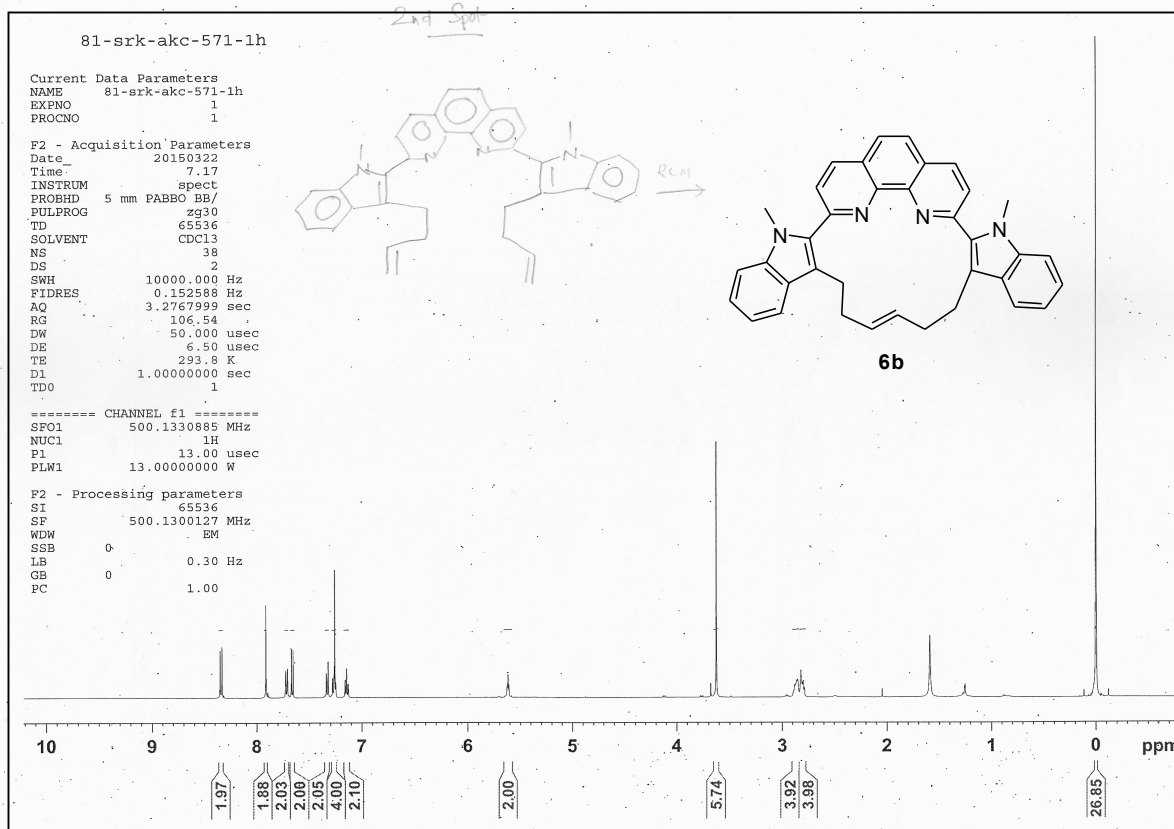
1H and 13C NMR of compound 5



1H and 13C NMR of compound 6a



1H and 13C NMR of compound 6b



X-ray crystallographic data and refinement parameters for **6a** (CCDC 1419802)

Bond precision:	C-C = 0.0177Å	Wavelength= 0.71070	
Cell:	a = 11.084 (5)	b = 28.328 (14)	c = 8.717 (4)
	$\alpha = 90$	$\beta = 90$	$\gamma = 90$
Temperature:	100 K		
	Calculated	Reported	
Volume	2737 (2)	2737 (2)	
Space group	p n c 2	p n c 2	
Hall group	P 2 -2bc	P 2 -2bc	
Moiety formula	C ₃₆ H ₃₀ N ₄	C ₃₆ H ₃₀ N ₄	
Sum formula	C ₃₆ H ₃₀ N ₄	C ₃₆ H ₃₀ N ₄	
Mr	518.64	518.64	
D _x , g cm ⁻³	1.259	1.259	
Z	4	4	
Mu (mm ⁻¹)	0.075	0.075	
F ₀₀₀	1096.0	1096.0	
F ₀₀₀ '	1096.37		
h, k, lmax	13, 33, 10	13, 33, 10	
N _{ref}	4826 [2590]	4789	
T _{min} , T _{max}	0.990, 0.993	0.923, 0.948	
T _{min} '	0.989		
Correction method = not given			
Data completeness = 1.85/0.99	Theta (max) = 24.998		
R(reflections) = 0.1002 (4432)	wR2(reflections) = 0.2233 (4789)		
S = 1.176	N _{par} = 363		

X-ray crystallographic data and refinement parameters for **6b** (CCDC 1419803)

Bond precision:	C-C = 0.0044Å	Wavelength= 1.54190	
Cell:	a = 30.190 (6)	b = 8.6781 (17)	c = 20.520 (4)
	$\alpha = 90$	$\beta = 90$	$\gamma = 90$
Temperature:	100 K		
	Calculated	Reported	
Volume	5376.1 (18)	5376.1 (19)	
Space group	p b c n	p b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C ₃₆ H ₃₀ N ₄	C ₃₆ H ₃₀ N ₄	
Sum formula	C ₃₆ H ₃₀ N ₄	C ₃₆ H ₃₀ N ₄	
Mr	518.64	518.66	
D _x ,g cm ⁻³	1.282	1.282	
Z	8	8	
Mu (mm-1)	0.587	0.588	
F000	2192.0	2192.0	
F000'	2197.79		
h, k, lmax	36, 10, 24	36, 10, 24	
Nref	4941	4927	
Tmin, Tmax	0.919, 0.948	0.923, 0.948	
Tmin'	0.916		
Correction method = Reported T Limits:	Tmin=0.923	Tmax=0.948	
AbsCorr = Numerical			
Data completeness = 0.997	Theta (max) = 68.320		
R(reflections) = 0.0767 (4565)	wR2(reflections) = 0.1918 (4927)		
S = 1.070	Npar = 361		