

Synthesis, X-ray Diffraction and Computational Druglikeness Evaluation of New Pyrrolo[1,2-*a*][1,10]Phenanthrolines Bearing a 9-Cyano Group

Mihaela Cristea ¹, Marcel Mirel Popa ^{1,*}, Sergiu Shova ², Maria Gdaniec ³, Amalia Stefaniu ⁴, Constantin Draghici ¹, Mihai Raduca ^{1,5}, Nicoleta Doriană Banu ¹ and Florea Dumitrascu ^{1,*}

- ¹ "C. D. Nenițescu" Institute of Organic and Supramolecular Chemistry, Romanian Academy, 202 B Splaiul Independenței, 060023 Bucharest, Romania; mihcris2012@yahoo.ro (M.C.); cst_drag@yahoo.com (C.D.); fiidemn@gmail.com (M.R.); doriana.banu@yahoo.com (N.D.B.)
- ² Department of Inorganic Polymers, Petru Poni Institute of Macromolecular Chemistry, Aleea Grigore Ghica Vodă nr. 41A, 700487 Iași, Romania; shova@icmpp.ro
- ³ Faculty of Chemistry, Adam Mickiewicz University, 61-614 Poznań, Poland; magdan@amu.edu.pl
- ⁴ National Institute of Chemical Pharmaceutical Research and Development—ICCF, 112 Vitan Av., 031299 Bucharest, Romania; astefaniu@gmail.com
- ⁵ Inorganic Chemistry Department, Faculty of Chemistry, University of Bucharest, Regina Elisabeta Blvd., 4-12, 030018 Bucharest, Romania
- * Correspondence: mirelupb@gmail.com (M.M.P.); fdumitra@yahoo.com (F.D.)

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Table S1. Bond distances (Å) and angles (°).

Compound 5a		Compound 5bHT		5bLT			Compound 5c	
Bond distances (Å)		Bond distances (Å)		Bond distances (Å)			Bond distances (Å)	
				Molecule	A	B		
O1-C17	1.2270(15)	O1-C1	1.216(3)	O1-C1	1.223(3)	1.222(3)	O1-C17	1.2189(17)
N1-C1	1.3196(17)	N1-C14	1.311(4)	N1-C14	1.317(4)	1.319(4)	O2-N4	1.2285(17)
N1-C12	1.3604(16)	N1-C15	1.358(4)	N1-C15	1.360(4)	1.357(4)	O3-N4	1.2297(16)
N2-C10	1.3938(16)	N2-C2	1.400(3)	N2-C2	1.405(3)	1.393(4)	N1-C1	1.3210(18)
N2-C11	1.4056(16)	N2-C5	1.387(3)	N2-C5	1.392(3)	1.396(4)	N1-C12	1.3602(18)
N2-C15	1.3961(16)	N2-C16	1.401(3)	N2-C16	1.403(3)	1.405(4)	N2-C10	1.3907(17)
N3-C16	1.1487(19)	N3-C17	1.148(3)	N3-C17	1.149(4)	1.150(4)	N2-C11	1.3968(17)
C1-C2	1.4055(19)	C1-C2	1.482(4)	C1-C2	1.483(4)	1.484(4)	N2-C15	1.4006(17)
C2-C3	1.3665(19)	C1-C18	1.481(4)	C1-C18	1.491(4)	1.492(4)	N3-C16	1.1493(19)
C3-C4	1.4099(19)	C2-C3	1.368(3)	C2-C3	1.366(4)	1.371(4)	N4-C21	1.4728(18)
C4-C5	1.4217(18)	C3-C4	1.403(4)	C3-C4	1.417(4)	1.404(4)	C1-C2	1.405(2)
C4-C12	1.4218(18)	C4-C5	1.387(4)	C4-C5	1.395(4)	1.398(4)	C2-C3	1.362(2)
C5-C6	1.3566(19)	C4-C17	1.418(4)	C4-C17	1.418(4)	1.425(4)	C3-C4	1.414(2)
C6-C7	1.4305(18)	C5-C6	1.409(4)	C5-C6	1.408(4)	1.407(4)	C4-C5	1.420(2)
C7-C8	1.4341(18)	C6-C7	1.338(4)	C6-C7	1.352(4)	1.345(5)	C4-C12	1.4200(19)
C7-C11	1.4007(18)	C7-C8	1.421(4)	C7-C8	1.428(4)	1.430(5)	C5-C6	1.357(2)
C8-C9	1.3510(19)	C8-C9	1.418(4)	C8-C9	1.422(4)	1.430(5)	C6-C7	1.428(2)
C9-C10	1.4148(18)	C8-C16	1.399(4)	C8-C16	1.399(4)	1.398(4)	C7-C8	1.430(2)
C10-C13	1.3918(18)	C9-C10	1.346(5)	C9-C10	1.359(4)	1.351(6)	C7-C11	1.4015(19)
C11-C12	1.4327(18)	C10-C11	1.417(5)	C10-C11	1.414(4)	1.420(5)	C8-C9	1.352(2)
C13-C14	1.4103(19)	C11-C12	1.393(5)	C11-C12	1.415(4)	1.408(5)	C9-C10	1.4149(19)
C13-C16	1.4277(19)	C11-C15	1.423(4)	C11-C15	1.420(4)	1.424(4)	C10-C13	1.394(2)
C14-C15	1.3728(18)	C12-C13	1.353(5)	C12-C13	1.360(5)	1.362(6)	C11-C12	1.4330(19)
C15-C17	1.4826(18)	C13-C14	1.417(5)	C13-C14	1.392(4)	1.398(5)	C13-C14	1.412(2)
C17-C18	1.4849(17)	C15-C16	1.420(4)	C15-C16	1.429(4)	1.432(4)	C13-C16	1.426(2)
C18-C19	1.3956(18)	C18-C19	1.384(4)	C18-C19	1.389(4)	1.389(4)	C14-C15	1.3719(19)
C18-C23	1.3950(18)	C18-C23	1.381(4)	C18-C23	1.397(4)	1.389(4)	C15-C17	1.4821(19)
C19-C20	1.3831(18)	C19-C20	1.377(4)	C19-C20	1.386(4)	1.377(4)	C17-C18	1.4946(19)
C20-C21	1.3972(19)	C20-C21	1.387(4)	C20-C21	1.397(4)	1.396(4)	C18-C19	1.3941(19)
C21-C22	1.3938(19)	C21-C22	1.390(4)	C21-C22	1.395(4)	1.395(4)	C18-C23	1.3974(19)
C21-C24	1.5047(18)	C21-C24	1.483(3)	C21-C24	1.488(4)	1.486(4)	C19-C20	1.383(2)
C22-C23	1.3852(19)	C22-C23	1.377(4)	C22-C23	1.382(4)	1.383(4)	C20-C21	1.383(2)
		C24-C25	1.379(4)	C24-C25	1.392(4)	1.392(4)	C21-C22	1.387(2)
		C24-C29	1.380(4)	C24-C29	1.401(4)	1.391(4)	C22-C23	1.385(2)
		C25-C26	1.380(4)	C25-C26	1.386(4)	1.385(4)		
		C26-C27	1.367(4)	C26-C27	1.388(4)	1.381(5)		
		C27-C28	1.365(4)	C27-C28	1.383(4)	1.391(5)		
		C28-C29	1.374(4)	C28-C29	1.386(4)	1.383(4)		
		C11-C30	1.715(9)					
		C12-C30	2.025(12)					
C13-C30	1.745(10)							

X-Ray Crystallography

Table S1. Bond distances (Å) and angles (°). (contd.)

Compound 5a		Compound 5bHT		5bLT			Compound 5c	
Angles (°)		Angles (°)					Angles (°)	
				Molecule	A	B		
C1-N1-C12	118.25(11)	C14-N1-C15	118.7(3)	C14-N1-C15	117.6(3)	118.3(3)	C1-N1-C12	118.10(12)
C10-N2-C11	120.45(10)	C2-N2-C16	130.5(2)	C5-N2-C2	108.6(2)	108.6(2)	C10-N2-C11	121.05(11)
C10-N2-C15	108.64(10)	C5-N2-C2	108.8(2)	C5-N2-C16	120.5(2)	120.4(2)	C10-N2-C15	108.84(11)
C15-N2-C11	130.45(11)	C5-N2-C16	120.4(2)	C16-N2-C2	130.5(2)	130.7(2)	C11-N2-C15	129.94(11)
N1-C1-C2	123.87(12)	O1-C1-C2	119.8(2)	O1-C1-C2	120.5(3)	120.1(3)	O2-N4-O3	123.75(13)
C3-C2-C1	118.33(12)	O1-C1-C18	121.6(2)	O1-C1-C18	121.7(3)	121.7(3)	O2-N4-C21	118.04(12)
C2-C3-C4	120.04(12)	C18-C1-C2	118.2(2)	C2-C1-C18	117.2(2)	117.6(2)	O3-N4-C21	118.21(12)
C3-C4-C5	122.51(12)	N2-C2-C1	123.8(2)	N2-C2-C1	123.0(2)	124.0(2)	N1-C1-C2	123.64(14)
C3-C4-C12	117.24(11)	C3-C2-N2	107.2(2)	C3-C2-N2	107.9(2)	107.9(2)	C3-C2-C1	118.75(14)
C5-C4-C12	120.22(11)	C3-C2-C1	124.3(2)	C3-C2-C1	124.8(2)	123.5(3)	C2-C3-C4	119.88(13)
C6-C5-C4	120.31(12)	C2-C3-C4	108.7(2)	C2-C3-C4	108.3(2)	108.5(3)	C3-C4-C5	123.27(13)
C5-C6-C7	121.21(12)	C3-C4-C17	127.7(2)	C3-C4-C17	128.0(3)	127.8(3)	C3-C4-C12	117.00(13)
C6-C7-C8	120.21(11)	C5-C4-C3	107.9(2)	C5-C4-C3	107.8(2)	107.7(3)	C12-C4-C5	119.58(13)
C11-C7-C6	119.24(12)	C5-C4-C17	124.3(2)	C5-C4-C17	124.2(3)	124.4(3)	C6-C5-C4	120.37(13)
C11-C7-C8	120.46(12)	N2-C5-C6	120.1(2)	N2-C5-C4	107.3(2)	107.1(2)	C5-C6-C7	121.40(13)
C9-C8-C7	120.25(12)	C4-C5-N2	107.2(2)	N2-C5-C6	120.0(2)	120.1(3)	C6-C7-C8	121.74(13)
C8-C9-C10	119.63(12)	C4-C5-C6	132.5(3)	C4-C5-C6	132.7(3)	132.6(3)	C11-C7-C6	118.57(13)
N2-C10-C9	119.90(11)	C7-C6-C5	119.7(3)	C7-C6-C5	119.4(3)	119.7(3)	C11-C7-C8	119.65(13)
C13-C10-N2	107.42(11)	C6-C7-C8	120.3(3)	C6-C7-C8	120.5(3)	120.4(3)	C9-C8-C7	120.83(13)
C13-C10-C9	132.57(12)	C9-C8-C7	120.1(3)	C9-C8-C7	120.5(3)	120.7(3)	C8-C9-C10	119.49(13)
N2-C11-C12	122.25(11)	C16-C8-C7	120.8(2)	C16-C8-C7	120.2(3)	120.6(3)	N2-C10-C9	119.75(12)
C7-C11-N2	117.43(11)	C16-C8-C9	119.0(3)	C16-C8-C9	119.1(3)	118.6(3)	N2-C10-C13	107.07(11)
C7-C11-C12	120.08(11)	C10-C9-C8	121.1(3)	C10-C9-C8	121.2(3)	121.5(4)	C13-C10-C9	133.16(13)
N1-C12-C4	121.99(11)	C9-C10-C11	121.1(3)	C9-C10-C11	120.6(3)	120.8(3)	N2-C11-C7	117.78(12)
N1-C12-C11	119.52(11)	C10-C11-C15	119.4(3)	C10-C11-C12	123.0(3)	123.2(3)	N2-C11-C12	122.37(12)
C4-C12-C11	118.35(11)	C12-C11-C10	123.5(3)	C10-C11-C15	119.8(3)	119.7(3)	C7-C11-C12	119.66(12)
C10-C13-C14	107.60(11)	C12-C11-C15	117.0(3)	C12-C11-C15	117.3(3)	117.0(4)	N1-C12-C4	122.33(12)
C10-C13-C16	124.14(12)	C13-C12-C11	120.7(3)	C13-C12-C11	119.5(3)	120.1(3)	N1-C12-C11	119.03(12)
C14-C13-C16	128.23(12)	C12-C13-C14	118.6(3)	C12-C13-C14	118.9(3)	118.7(4)	C4-C12-C11	118.50(12)
C15-C14-C13	108.47(11)	N1-C14-C13	122.9(4)	N1-C14-C13	124.5(3)	123.7(4)	C10-C13-C14	108.12(12)
N2-C15-C17	123.73(11)	N1-C15-C11	122.0(3)	N1-C15-C11	122.3(3)	122.1(3)	C10-C13-C16	124.90(13)
C14-C15-N2	107.74(11)	N1-C15-C16	119.6(2)	N1-C15-C16	119.0(2)	119.6(3)	C14-C13-C16	126.86(13)
C14-C15-C17	125.09(11)	C16-C15-C11	118.3(3)	C11-C15-C16	118.7(3)	118.2(3)	C15-C14-C13	108.03(12)
N3-C16-C13	177.94(15)	N2-C16-C15	122.2(2)	N2-C16-C15	122.3(2)	121.8(3)	N2-C15-C17	122.32(11)
O1-C17-C15	120.14(11)	C8-C16-N2	117.1(2)	C8-C16-N2	117.5(2)	117.2(3)	C14-C15-N2	107.90(11)
O1-C17-C18	122.03(12)	C8-C16-C15	120.6(2)	C8-C16-C15	120.1(2)	120.8(3)	C14-C15-C17	126.33(12)
C15-C17-C18	117.29(11)	N3-C17-C4	179.4(3)	N3-C17-C4	178.9(3)	179.2(3)	N3-C16-C13	179.16(17)
C19-C18-C17	118.96(11)	C19-C18-C1	122.3(2)	C19-C18-C1	122.3(3)	119.2(3)	O1-C17-C15	120.21(12)
C23-C18-C17	122.22(11)	C23-C18-C1	119.6(2)	C19-C18-C23	118.8(3)	118.9(3)	O1-C17-C18	121.00(12)
C23-C18-C19	118.82(12)	C23-C18-C19	118.0(2)	C23-C18-C1	118.9(3)	121.9(3)	C15-C17-C18	118.69(11)
C20-C19-C18	120.56(12)	C20-C19-C18	120.7(3)	C20-C19-C18	120.6(3)	120.6(3)	C19-C18-C17	121.52(12)

C19-C20-C21	120.76(12)	C19-C20-C21	121.7(3)	C19-C20-C21	121.1(3)	121.2(3)	C19-C18-C23	119.78(12)
C20-C21-C24	120.95(12)	C20-C21-C22	117.1(2)	C20-C21-C24	121.2(3)	120.5(3)	C23-C18-C17	118.57(12)
C22-C21-C20	118.35(12)	C20-C21-C24	122.5(2)	C22-C21-C20	117.9(3)	117.7(3)	C20-C19-C18	120.37(13)
C22-C21-C24	120.69(12)	C22-C21-C24	120.3(2)	C22-C21-C24	120.9(3)	121.7(3)	C21-C20-C19	118.39(13)
C23-C22-C21	121.02(12)	C23-C22-C21	121.1(3)	C23-C22-C21	121.3(3)	121.1(3)	C20-C21-N4	118.08(13)
C22-C23-C18	120.31(12)	C22-C23-C18	121.3(3)	C22-C23-C18	120.3(3)	120.4(3)	C20-C21-C22	122.93(13)
		C25-C24-C21	121.1(2)	C25-C24-C21	121.3(3)	121.5(3)	C22-C21-N4	119.00(12)
		C25-C24-C29	117.1(3)	C25-C24-C29	118.0(3)	117.9(3)	C23-C22-C21	117.88(13)
		C29-C24-C21	121.8(2)	C29-C24-C21	120.6(3)	120.5(3)	C22-C23-C18	120.62(13)
		C24-C25-C26	121.3(3)	C26-C25-C24	121.1(3)	120.8(3)		
		C27-C26-C25	120.5(3)	C25-C26-C27	120.3(3)	120.8(3)		
		C28-C27-C26	119.1(3)	C28-C27-C26	119.4(3)	119.1(3)		
		C27-C28-C29	120.4(3)	C27-C28-C29	120.4(3)	119.9(3)		
		C28-C29-C24	121.7(3)	C28-C29-C24	120.8(3)	121.5(3)		
		Cl1-C30-Cl2	94.1(5)					
		Cl1-C30-Cl3	109.3(5)					
		Cl3-C30-Cl2	95.4(5)					

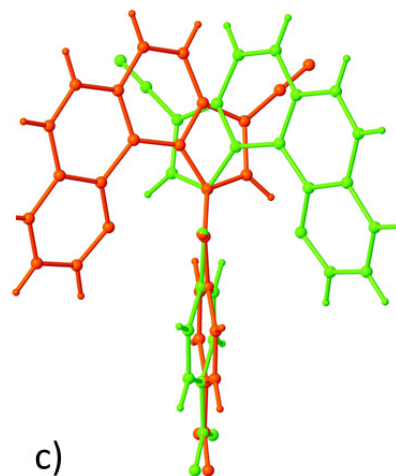
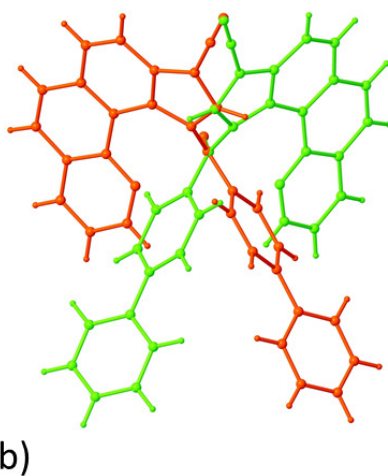
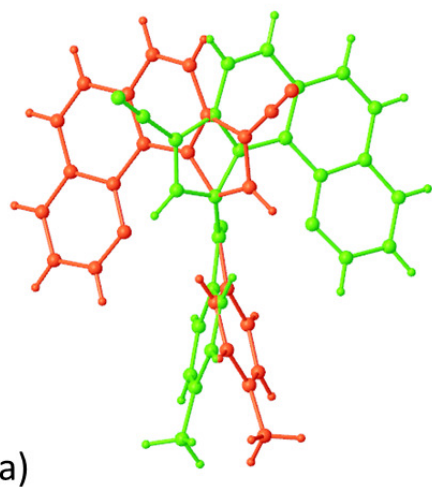


Figure S1. Overlaid molecules illustrating the helical chirality for **5a** (a), **5b** (b) and **5c** (c).

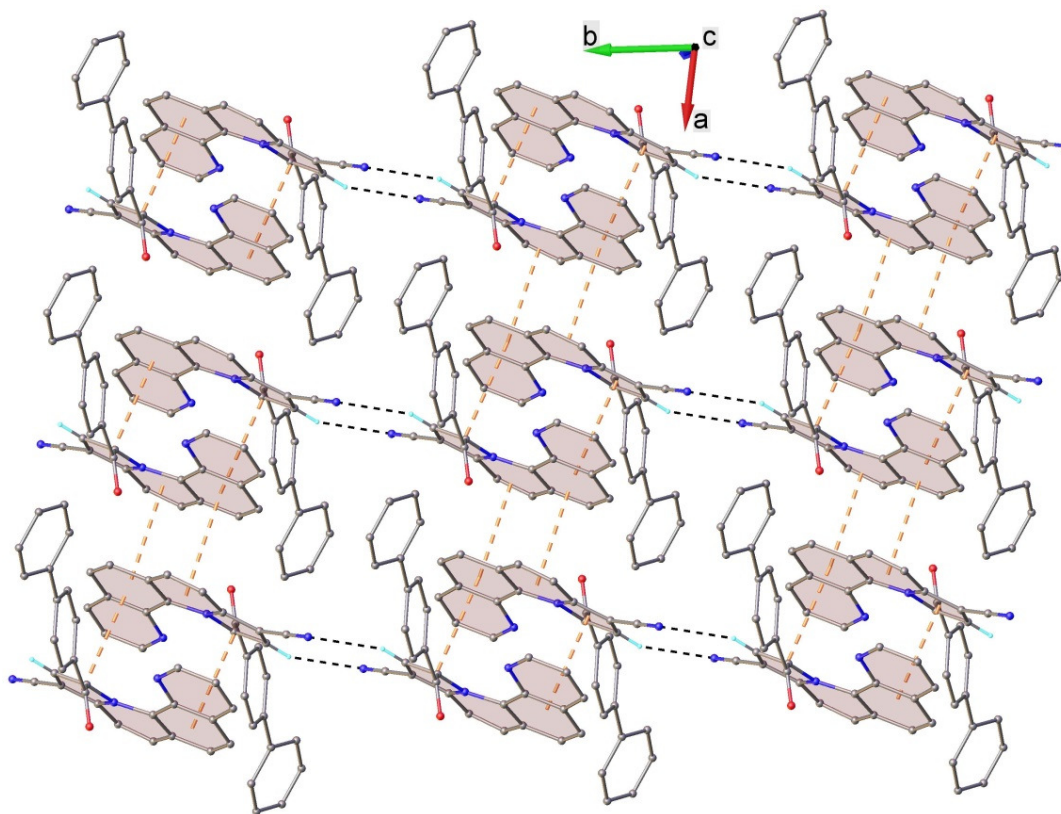
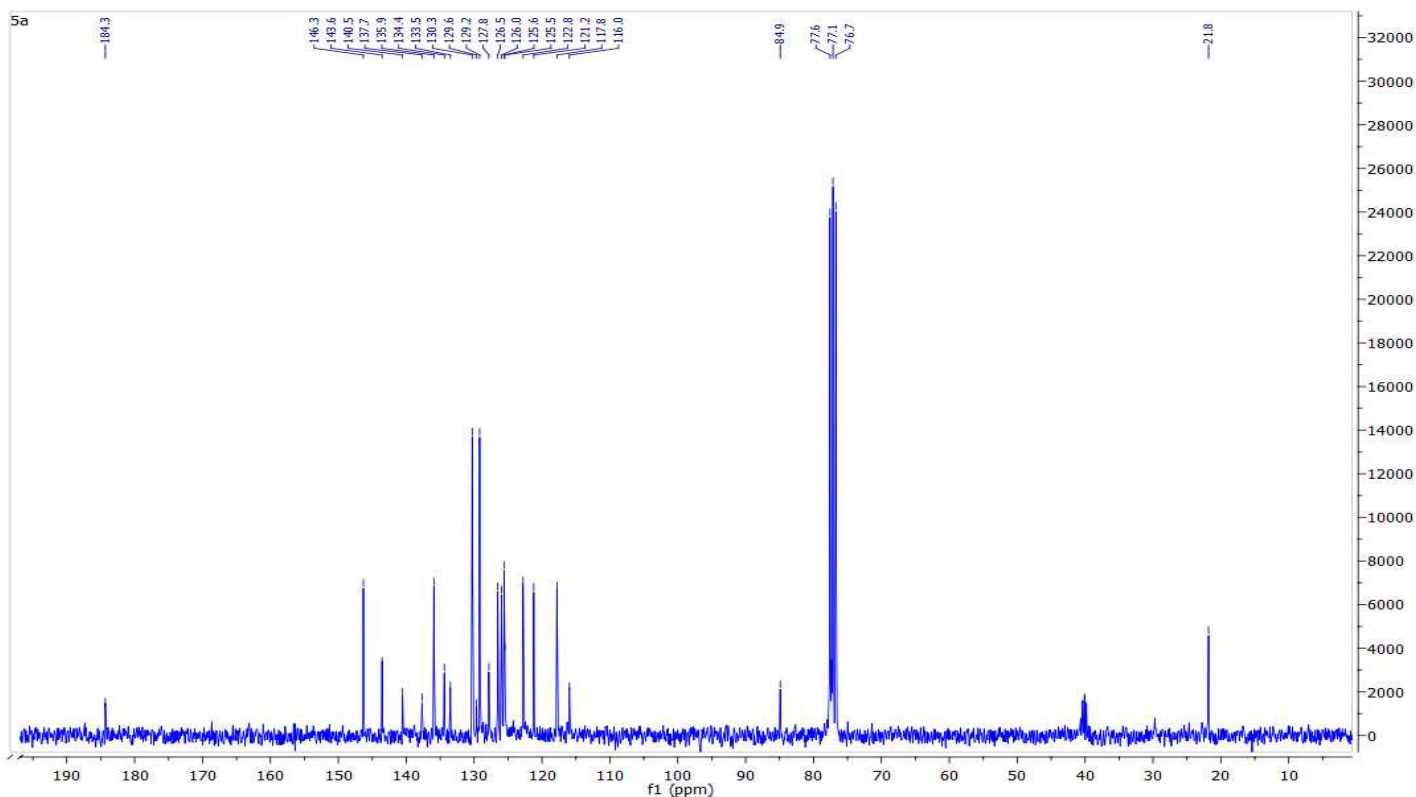
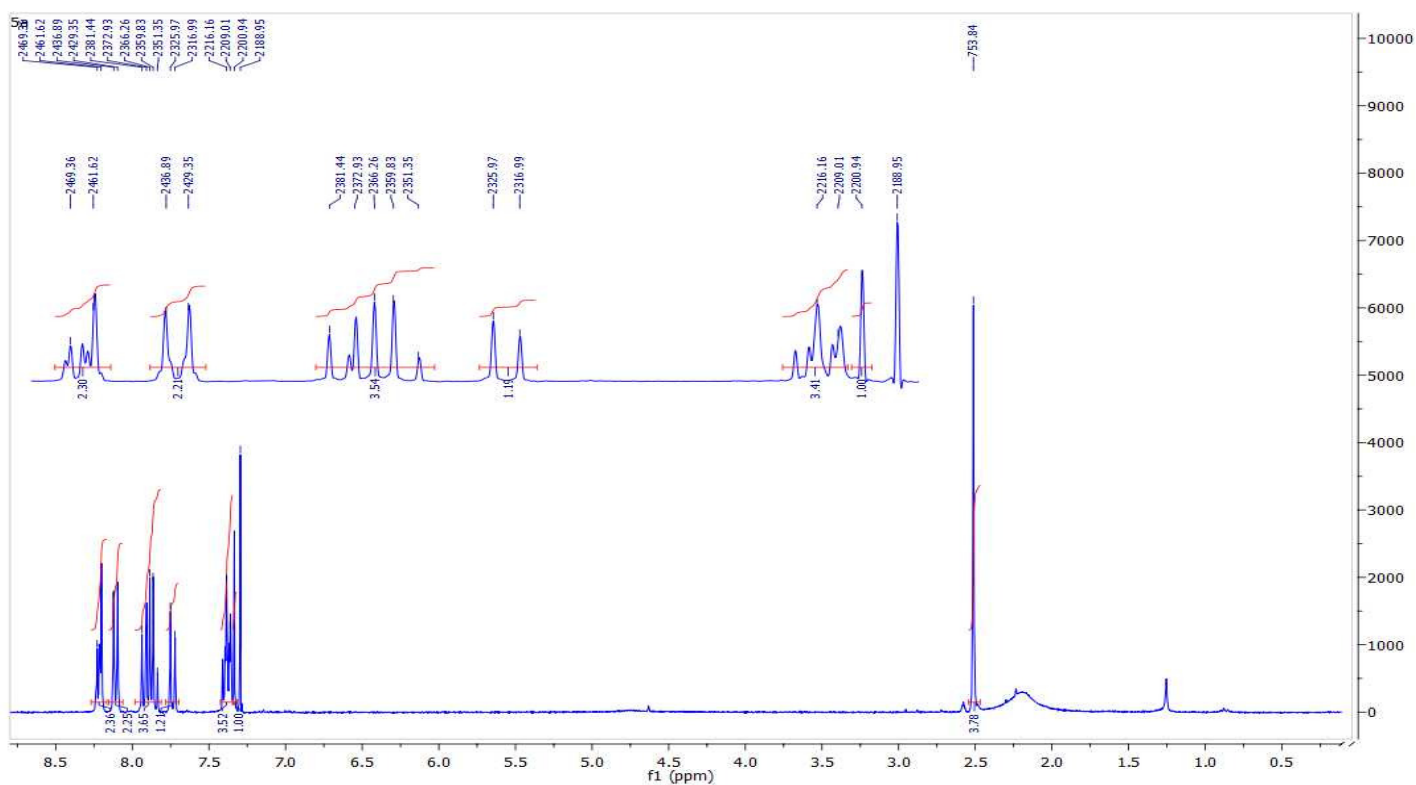


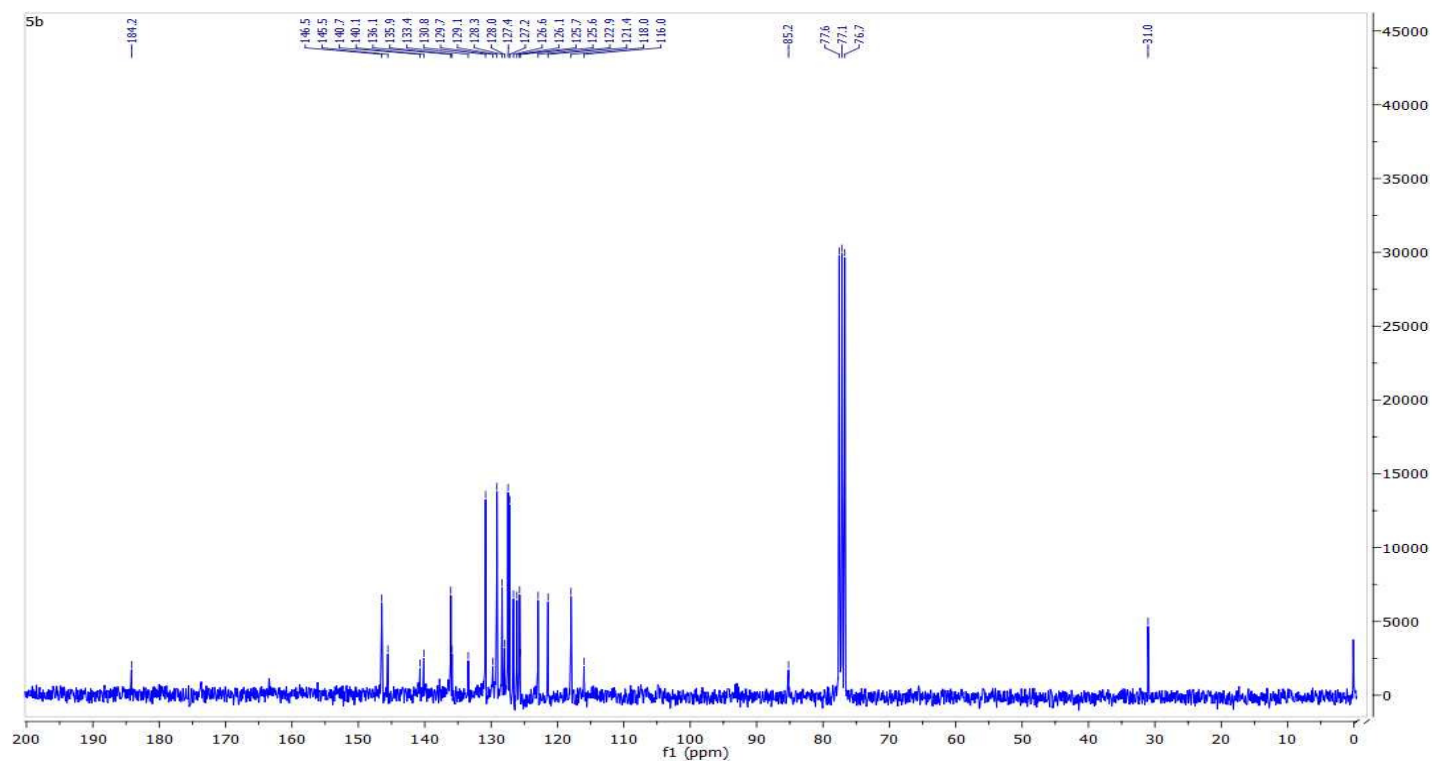
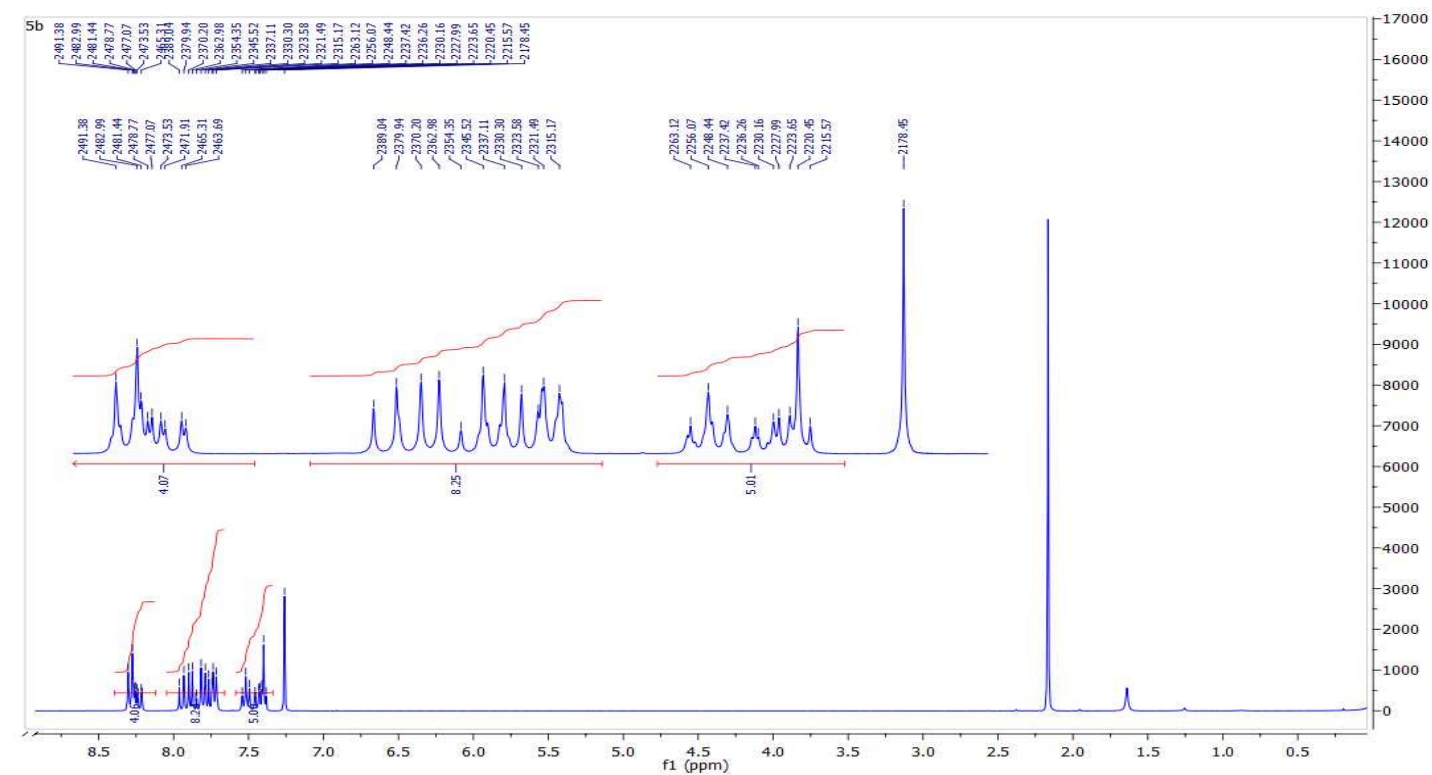
Figure S2. View of 2D supramolecular layer in the crystal structure **5b**. H bonds and centroid-to-centroid distances are shown in dashed black and orange lines, respectively

NMR Spectra

^1H and ^{13}C -NMR of compound 5a



¹H and ¹³C-NMR of compound 5b



^1H and ^{13}C -NMR of compound 5c

