Electronic Supplementary Information

Synthesis and Investigation of Electrical Properties of Novel Liquid-Crystal Phthalocyanines

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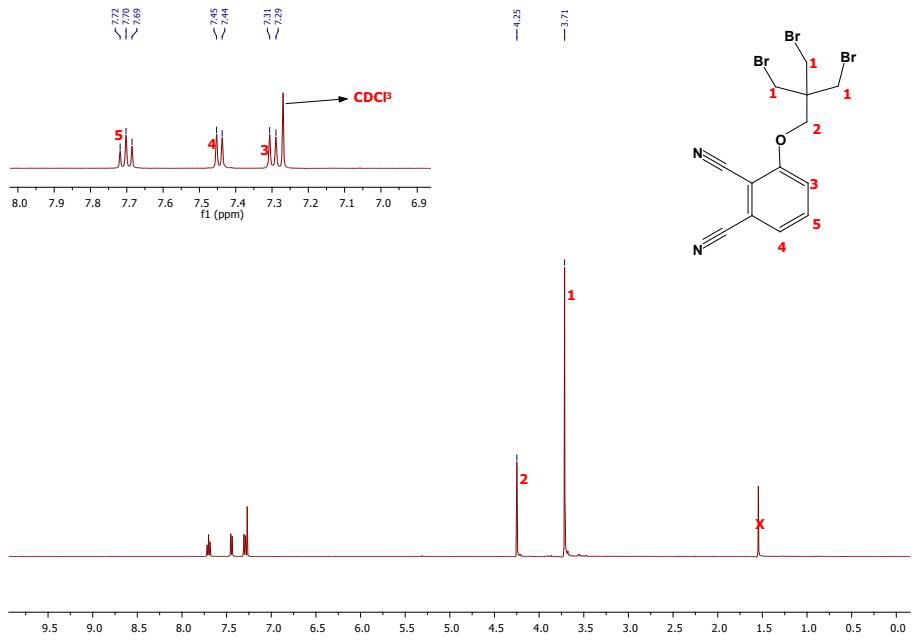

Figure S1. ^{1}H NMR spectrum of compound **4**

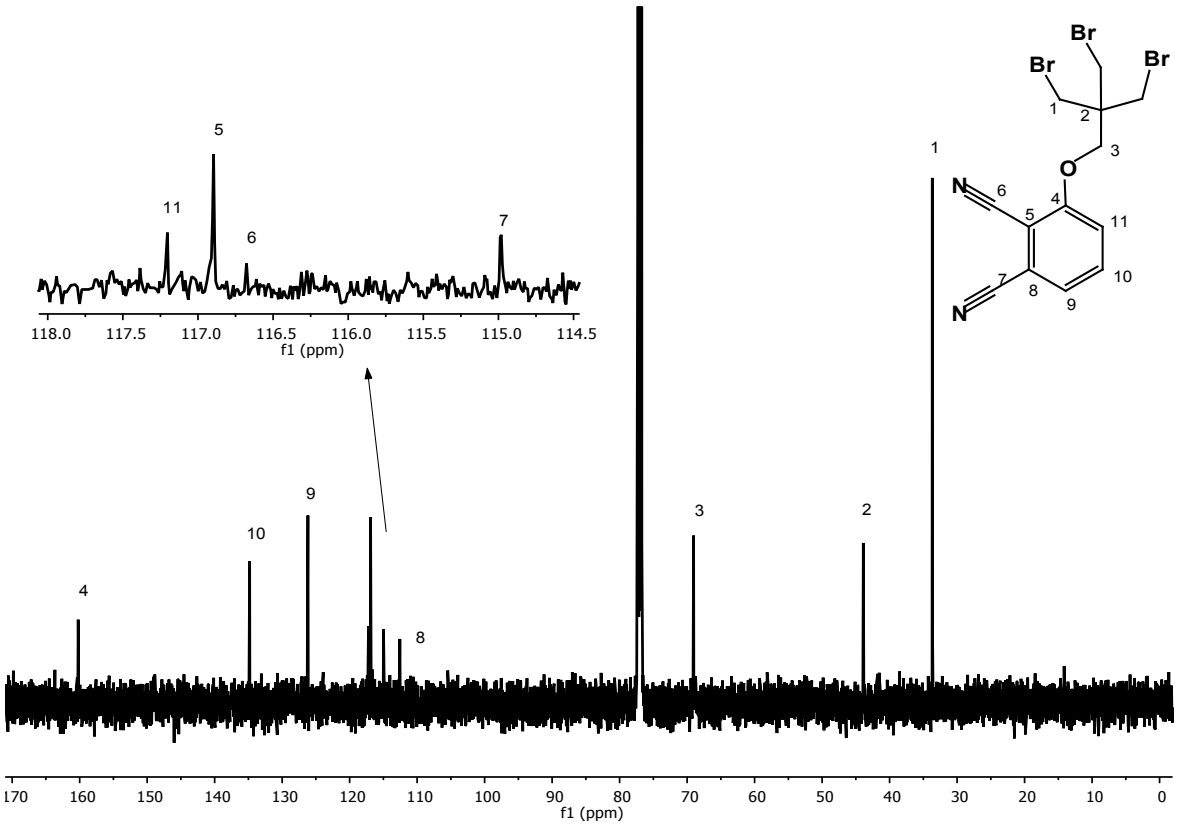

Figure S2. ^{13}C NMR spectrum of compound **4**

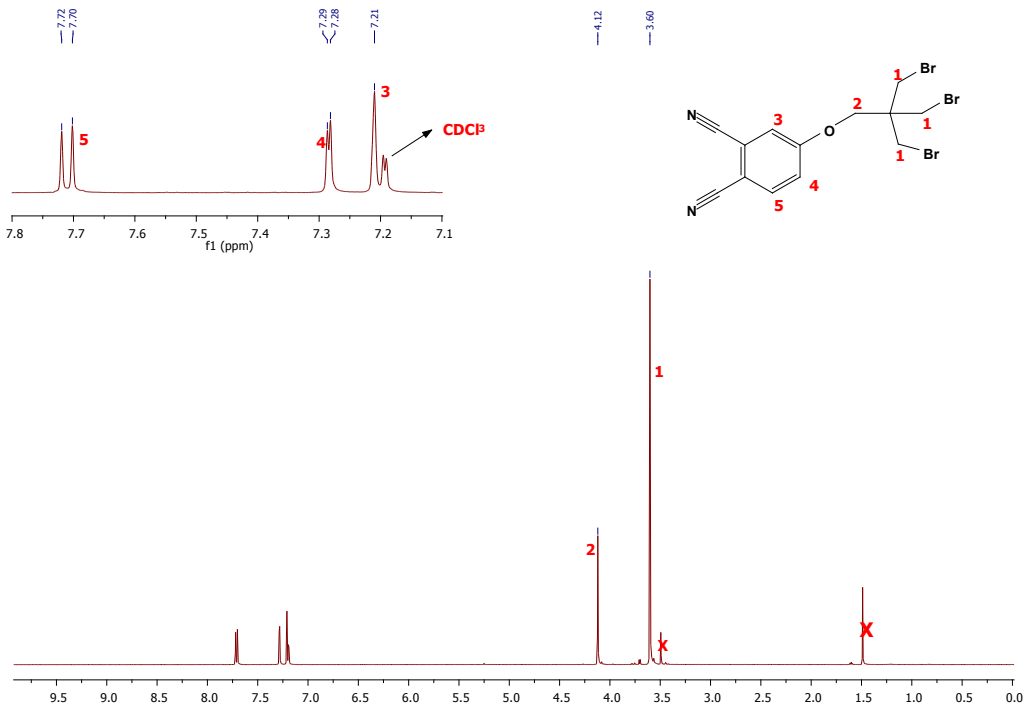

Figure S3. ^{1}H NMR spectrum of compound **5**

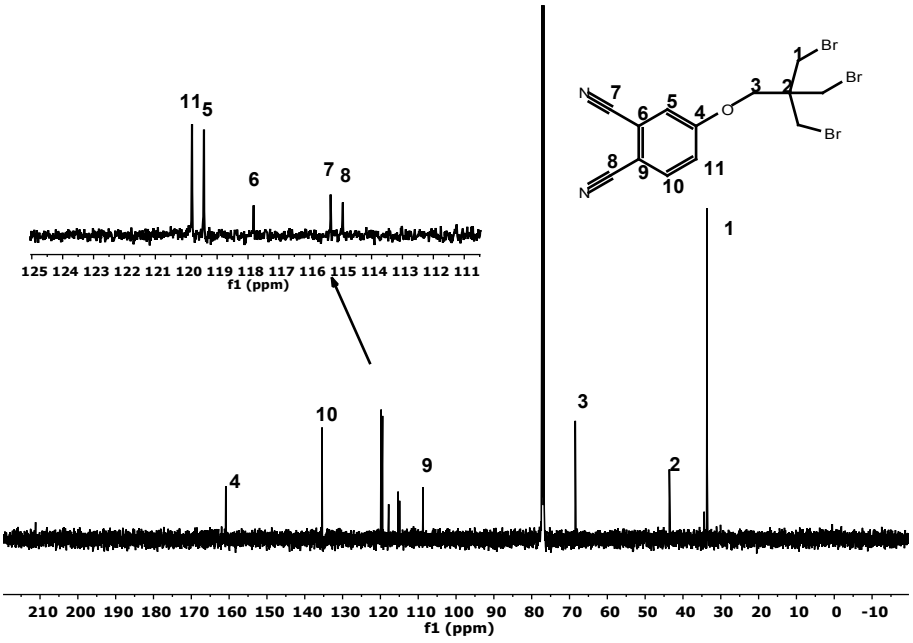

Figure S4. ^{13}C NMR spectrum of compound **5**

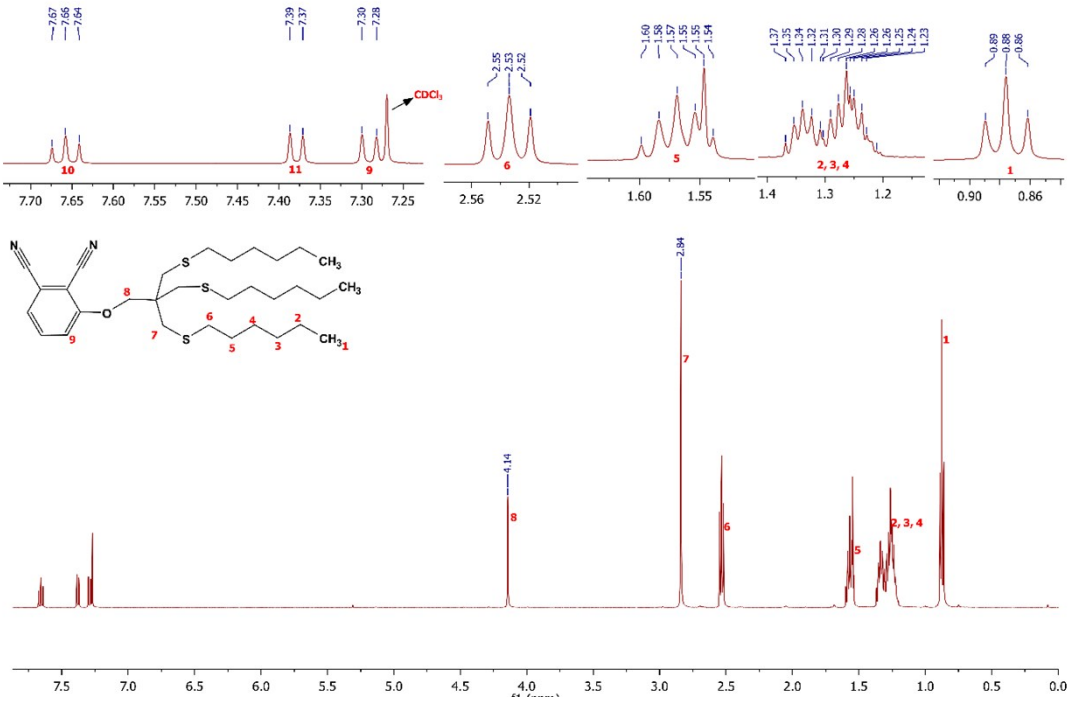

Figure S5. ^{1}H NMR spectrum of compound **6**

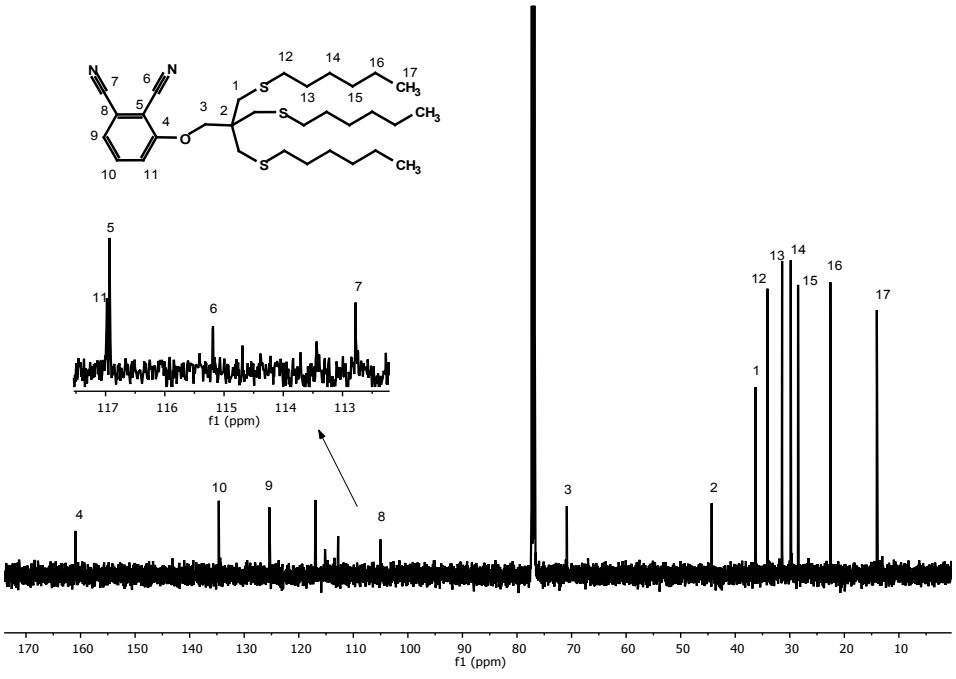

Figure S6. ^{13}C NMR spectrum of compound **6**

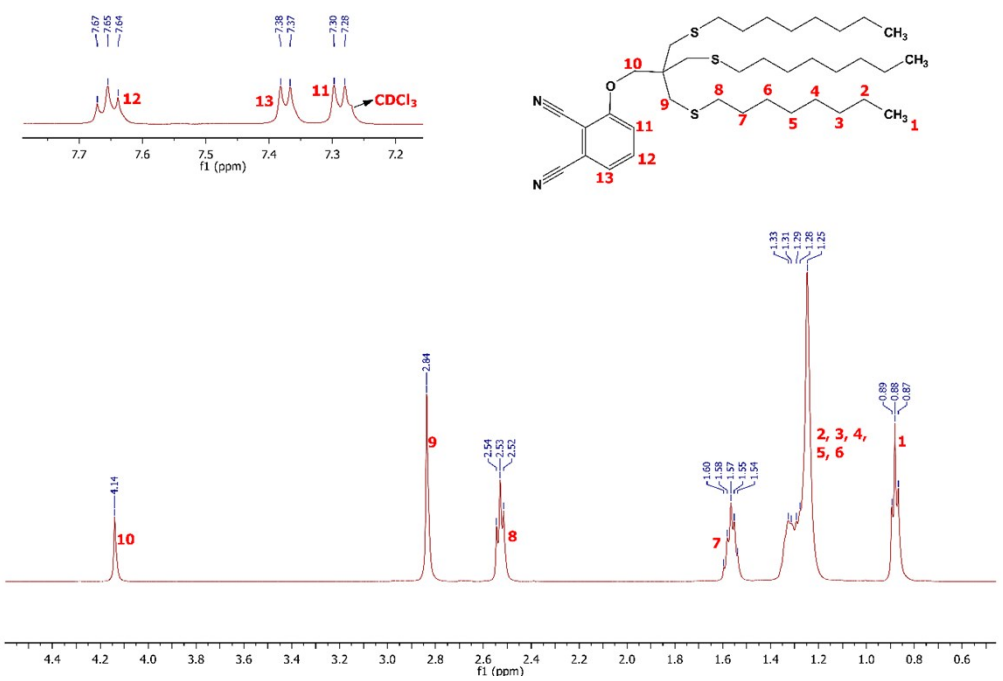

Figure S7. ^{1}H NMR spectrum of compound **7**

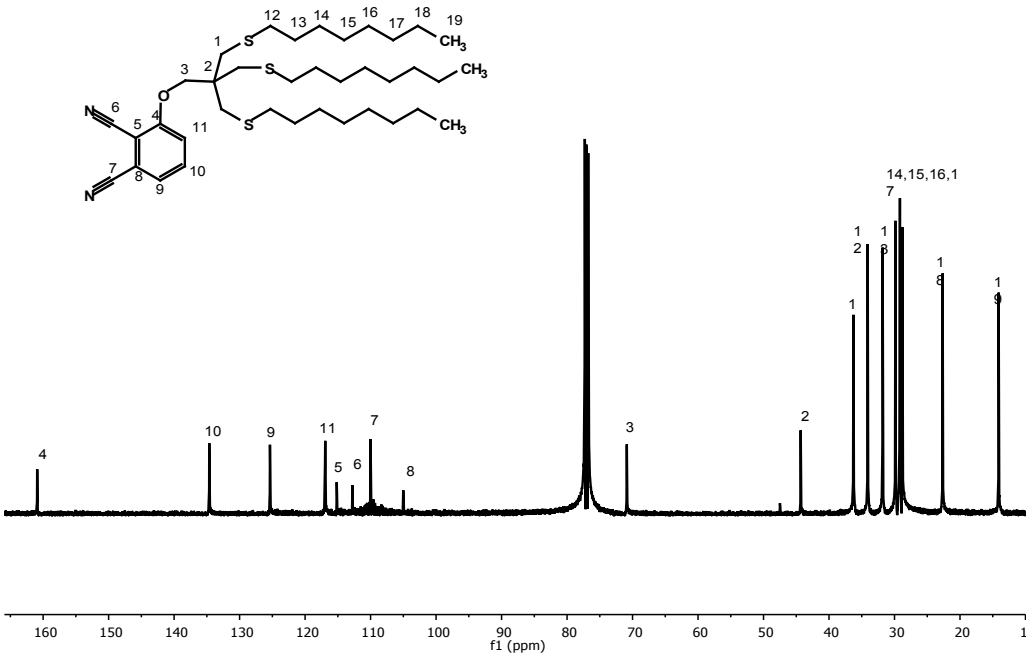

Figure S8. ^{13}C NMR spectrum of compound **7**

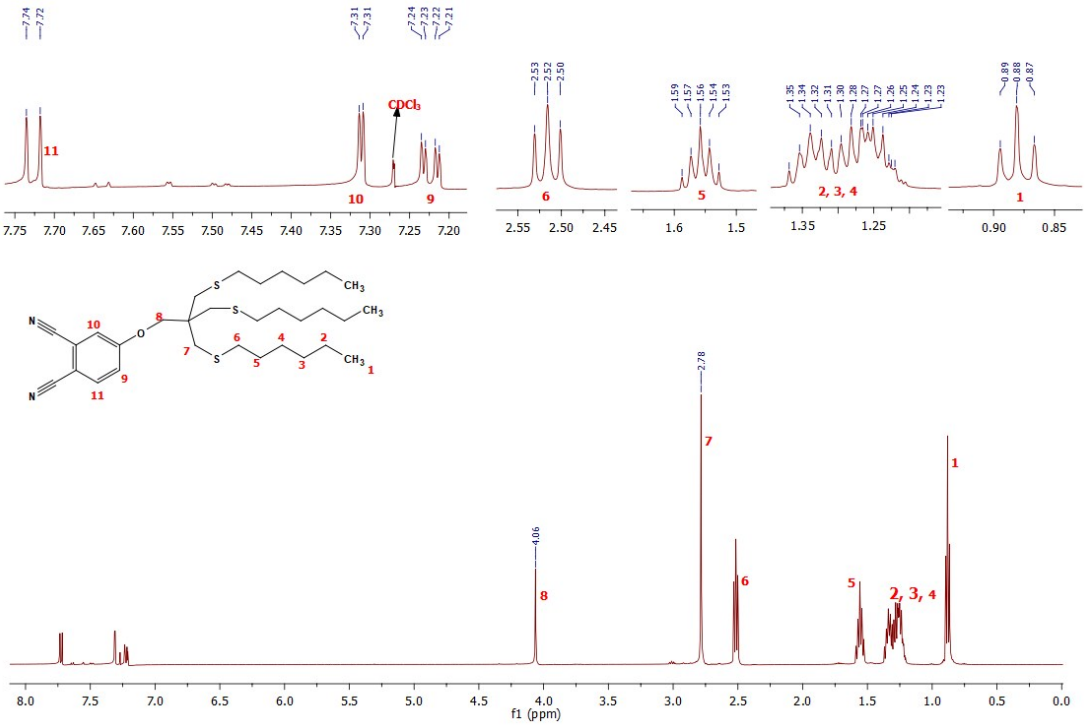

Figure S9. ^{1}H NMR spectrum of compound **8**

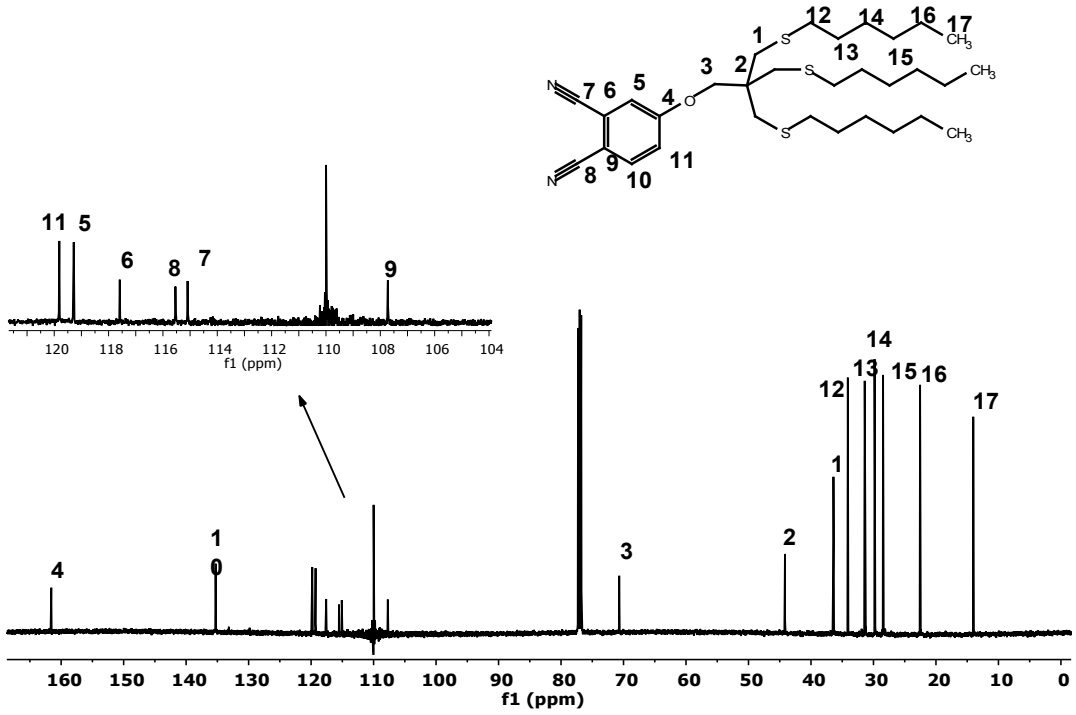

Figure S10. ^{13}C NMR spectrum of compound **8**

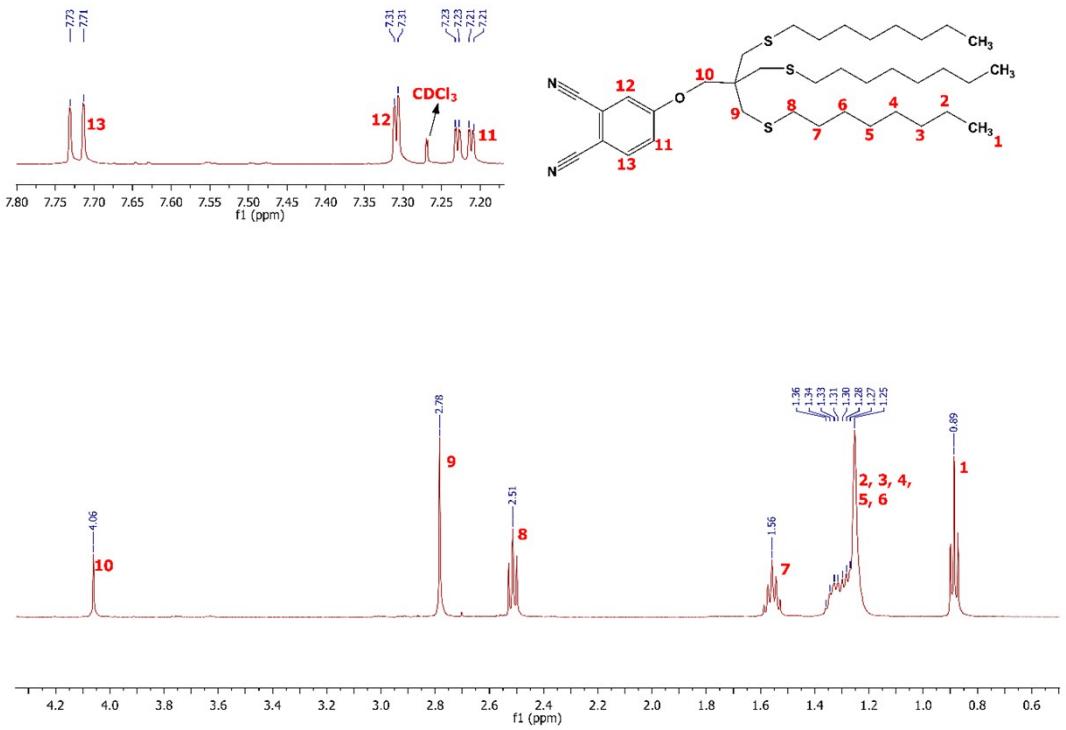

Figure S9. ^{1}H NMR spectrum of compound **9**

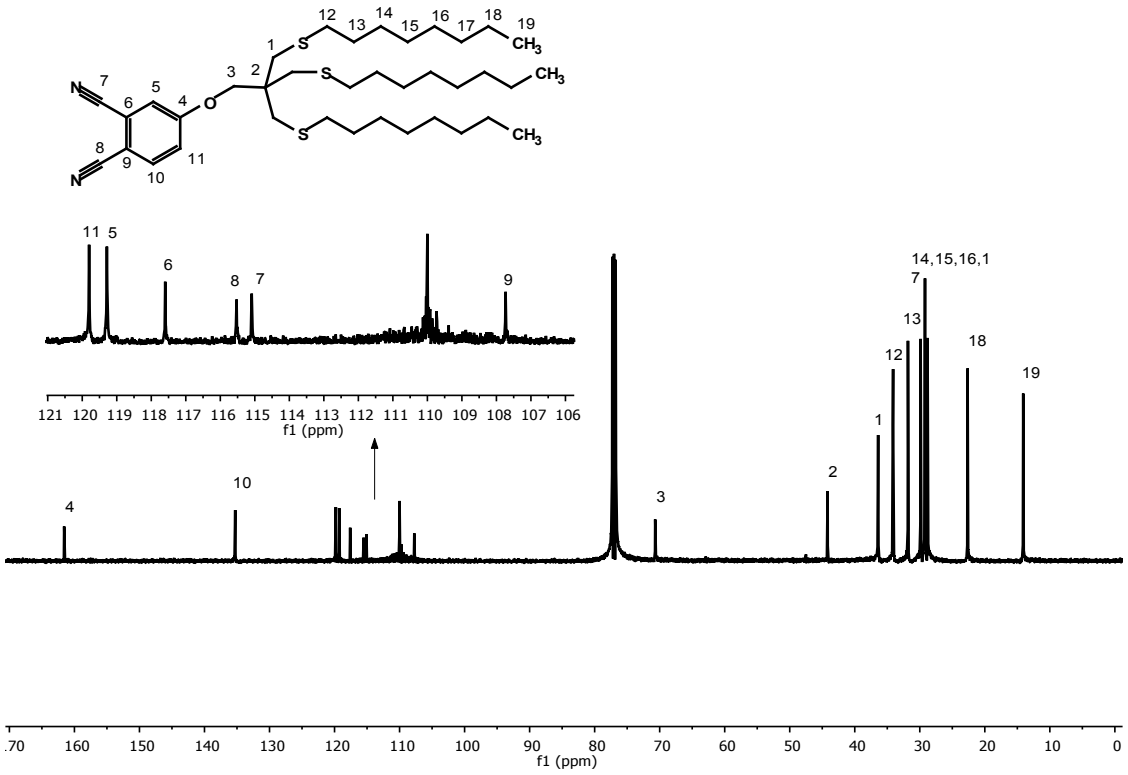

Figure S10. ^{13}C NMR spectrum of compound **9**

Table S1. Selected bond parameters for compounds **4** and **5**			
Bond Lengths (Å)			
4		**5**	
Br1-C11	1.962(9)	Br1-C11	1.929(5)
Br2-C12	1.954(10)	Br2-C12	1.939(5)
Br3-C13	1.954(11)	Br3-C13	1.952(5)
O1-C4	1.334(13)	O1-C1	1.346(6)
O1-C9	1.431(12)	O1-C9	1.444(6)
N1-C1	1.121(14)	N1-C7	1.135(6)
N2-C2	1.149(13)	N2-C8	1.138(7)
C1-C8	1.454(14)	C1-C2	1.388(6)
C2-C3	1.428(14)	C1-C6	1.402(7)
C3-C4	1.415(14)	C2-C3	1.380(7)
C3-C8	1.411(15)	C3-C4	1.398(6)
C4-C5	1.385(14)	C3-C7	1.448(7)
C5-C6	1.397(15)	C4-C5	1.386(7)
C6-C7	1.381(15)	C4-C8	1.435(7)
C7-C8	1.384(14)	C5-C6	1.368(7)
C10-C9	1.540(15)	C9-C10	1.510(6)
C10-C11	1.546(13)	C10-C11	1.527(6)
C10-C12	1.546(13)	C10-C12	1.524(6)
C10-C13	1.538(15)	C10-C13	1.523(6)
Bond Angles (°)			
C4-O1-C9	120.3(8)	C1-O1-C9	117.4(3)
N1-C1-C8	178.5(12)	N1-C7-C3	179.1(6)
N2-C2-C3	178.8(11)	N2-C4-C8	178.6(6)
C10-C11-Br1	112.5(7)	C10-C11-Br1	114.2(3)
C10-C12-Br2	113.7(7)	C10-C12-Br2	114.5(3)
C10-C13-Br3	114.3(7)	C10-C13-Br3	114.3(3)
Dihedral Angles (°)			
C4-O1-C9-C10	179.3(8)	C1-O1-O9-C10	178.0(5)
C9-C10-C11-Br1	57.4(10)	C9-C10-C11-Br1	57.0(5)
C9-C10-C12-Br2	58.9(10)	C9-C10-C12-Br2	-64.3(5)
C9-C10-C13-Br3	173.3(6)	C9-C10-C13-Br3	177.9(3)
C12-C10-C11-Br1	-64.2(10)	C12-C10-C11-Br1	177.8(3)
C11-C10-C12-Br2	-178.8(7)	C11-C10-C12-Br2	175.1(3)
C11-C10-C13-Br3	54.2(10)	C11-C10-C13-Br3	-61.1(5)
C13-C10-C11-Br1	173.1(7)	C13-C10-C11-Br1	-59.8(5)
C13-C10-C12-Br2	-59.1(11)	C13-C10-C12-Br2	53.4(5)
C12-C10-C13-Br3	-66.4(10)	C12-C10-C13-Br3	56.1(5)

Table S2 inter molecular interactions in the X-ray structures of **4**					
D–H···A	**D-H (Å)**	**H···A (Å)**	**D···A (Å)**	**DHA (°)**	**Symmetry code**
C2-H2···O1	0.93	2.47	3.384 (7)	168.4	1-x,1-y,1-z

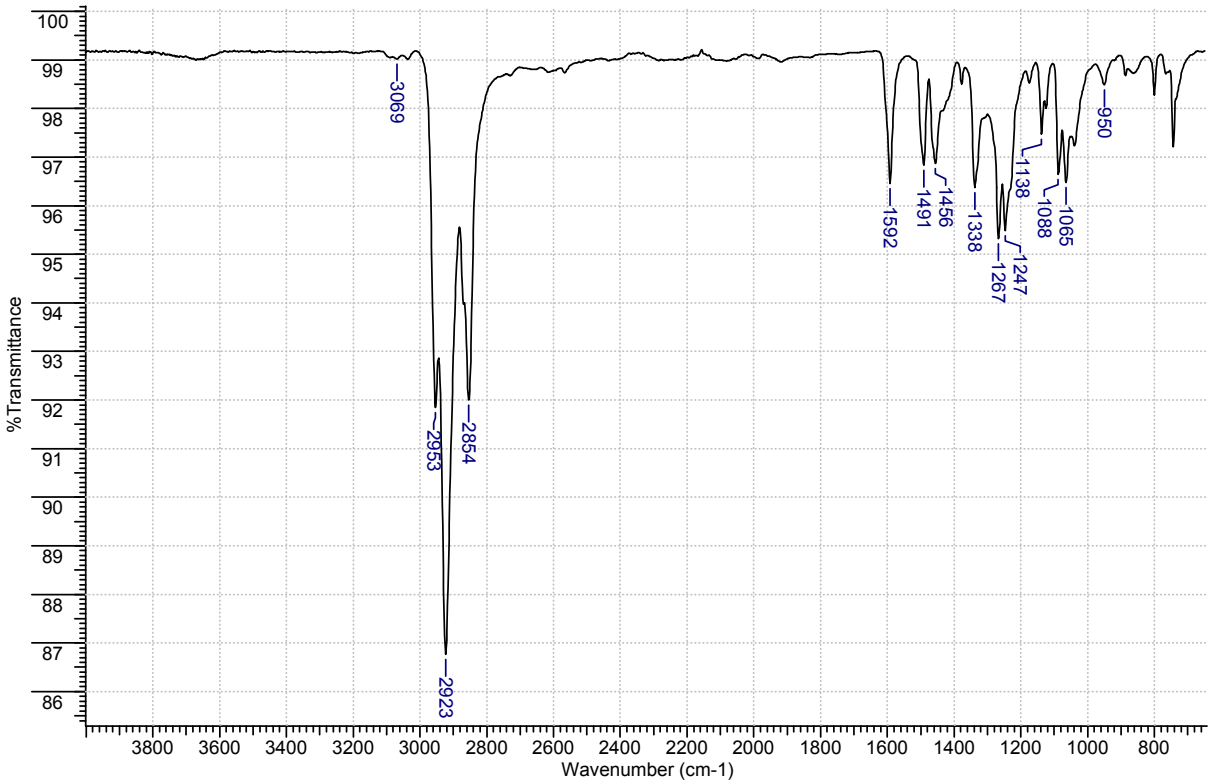

Figure S11. FT-IR spectrum of compound **10a**

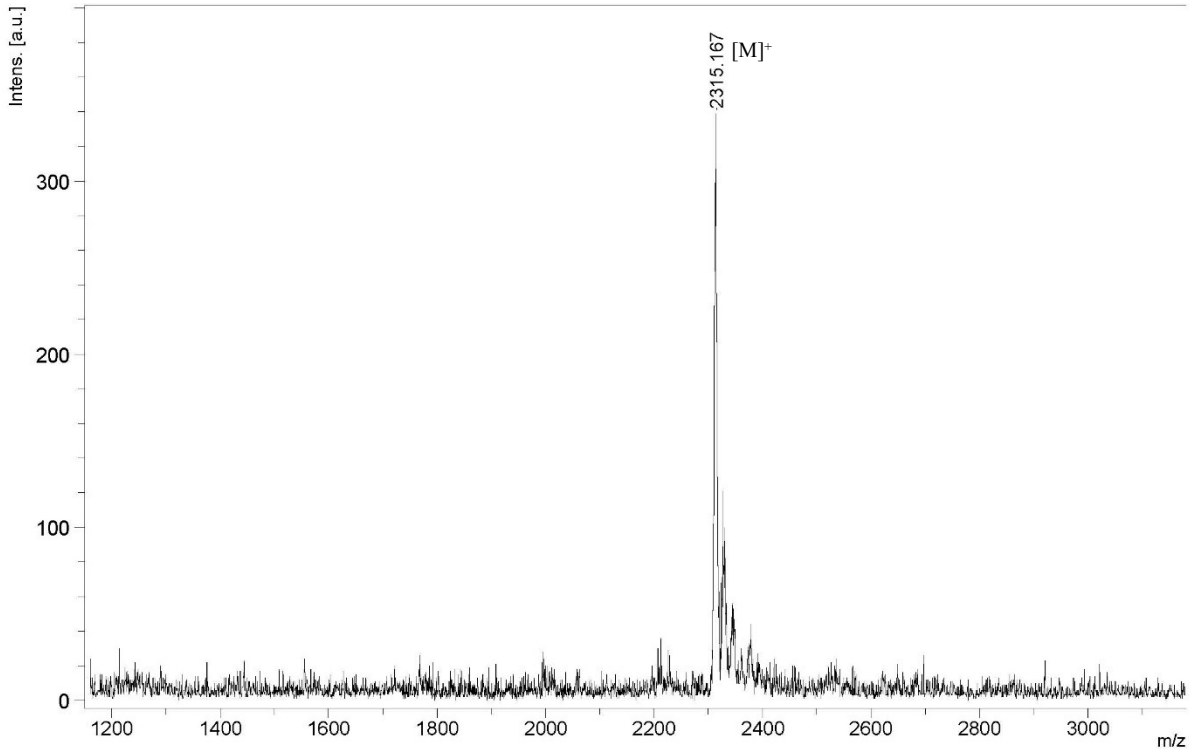

Figure S12. MALDI-TOF spectrum of compound **10a**

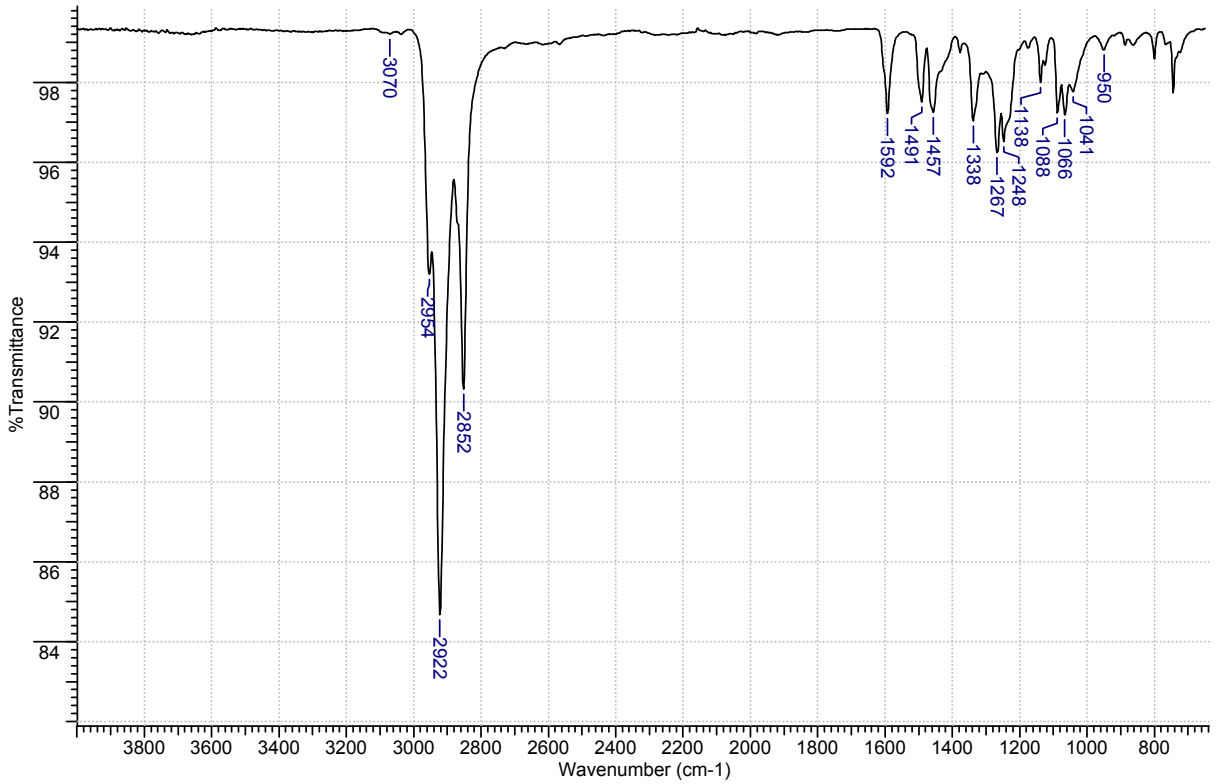

Figure S13. FT-IR spectrum of compound **10b**

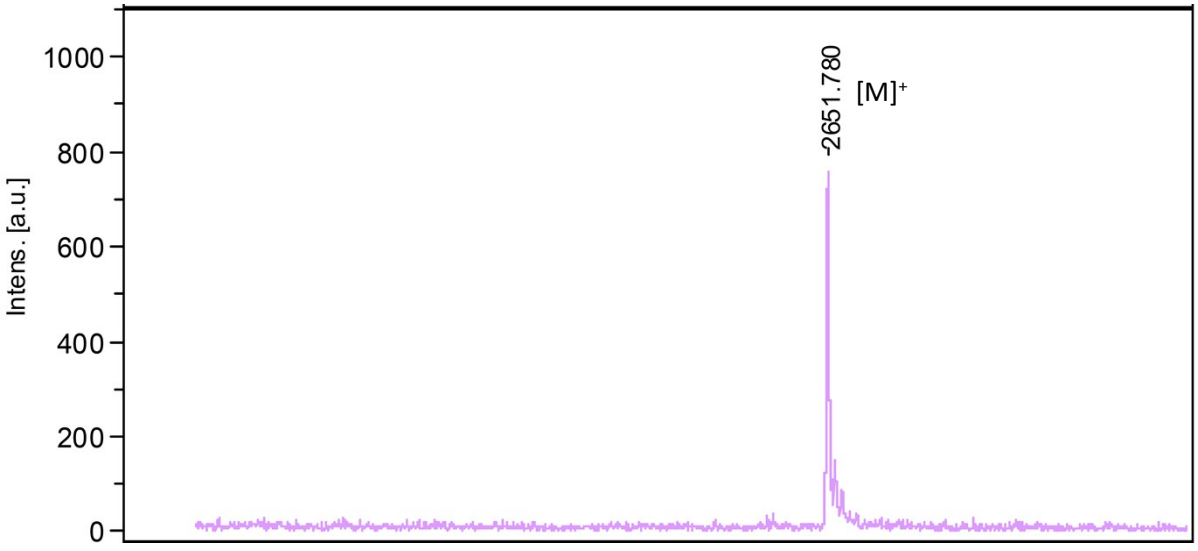

Figure S14. MALDI-TOF spectrum of compound **10b**

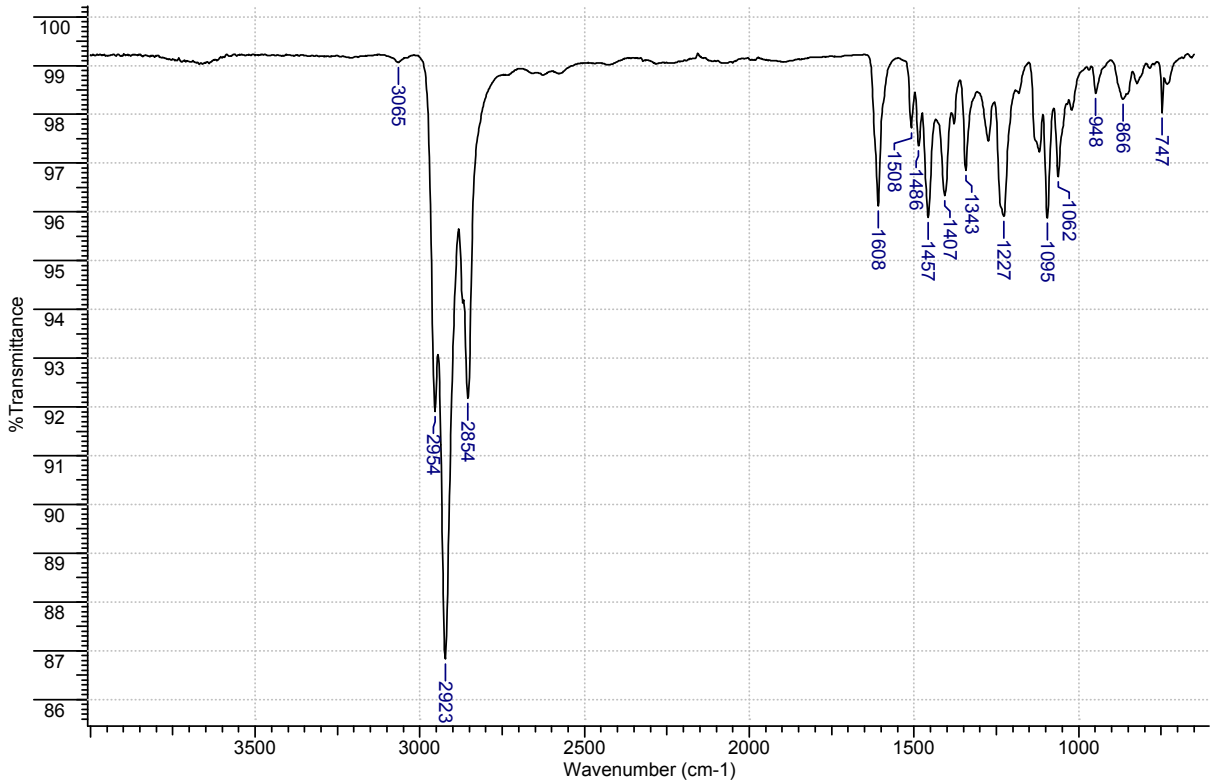

Figure S15. FT-IR spectrum of compound **11a**

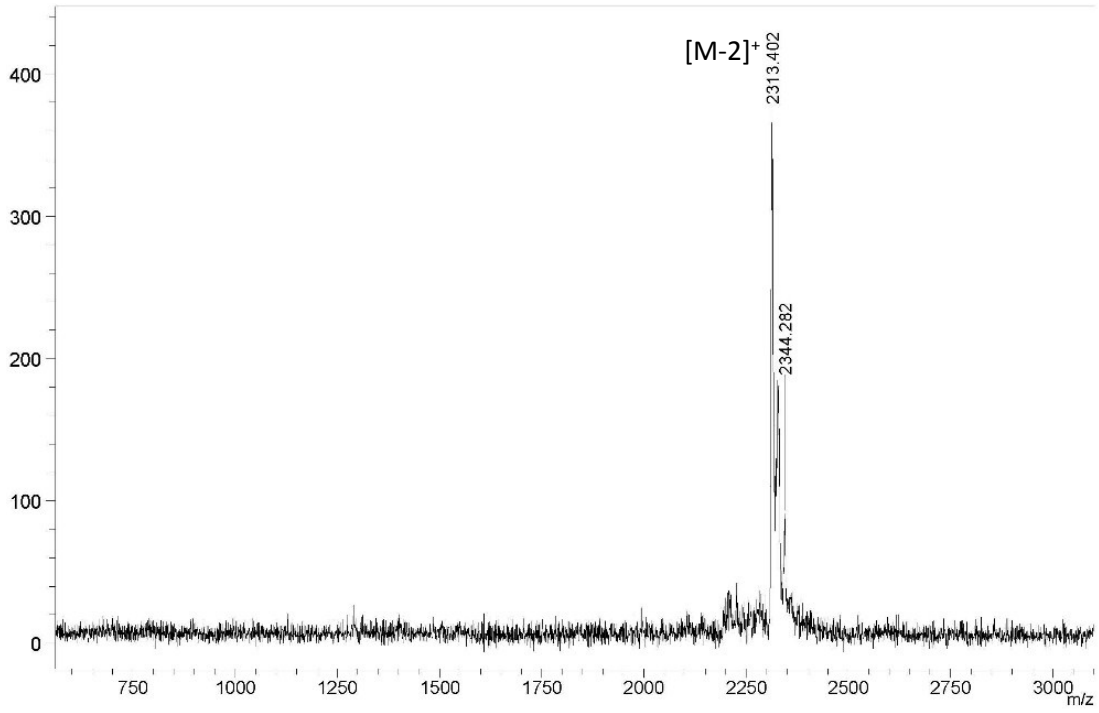

Figure S16. MALDI-TOF spectrum of compound **11a**

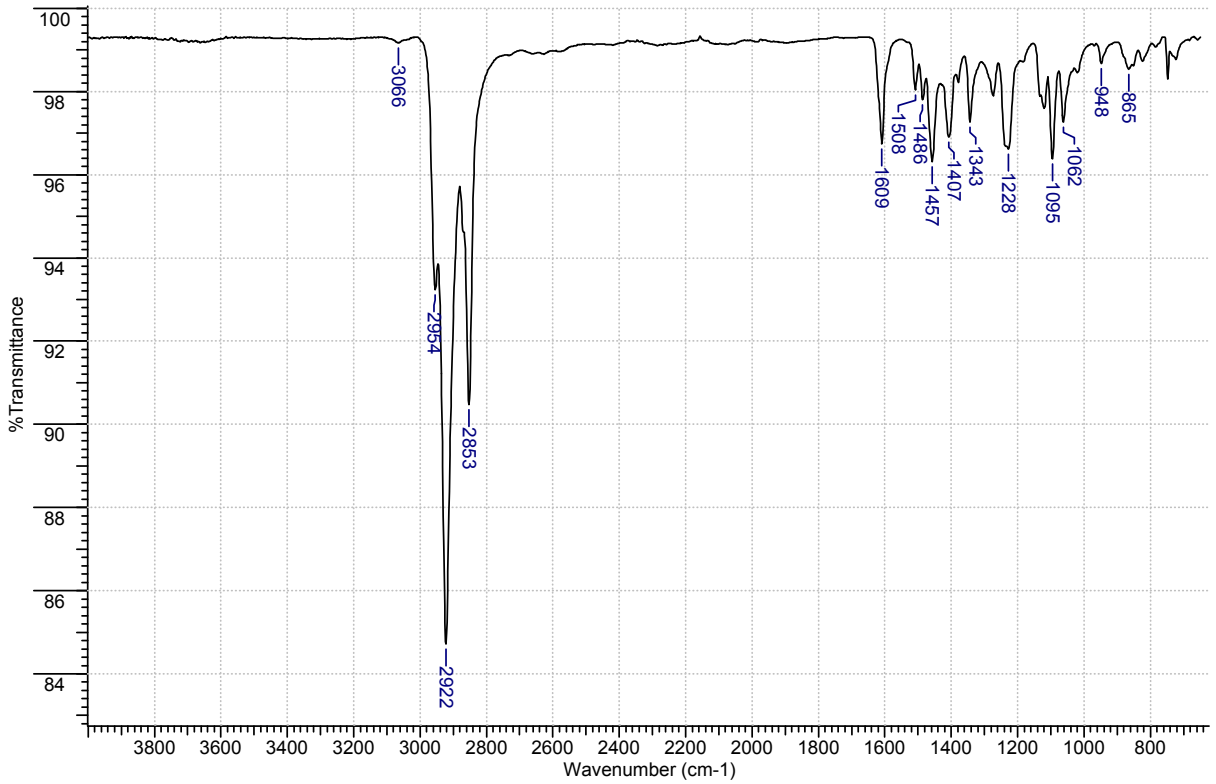

Figure S17. FT-IR spectrum of compound **11b**

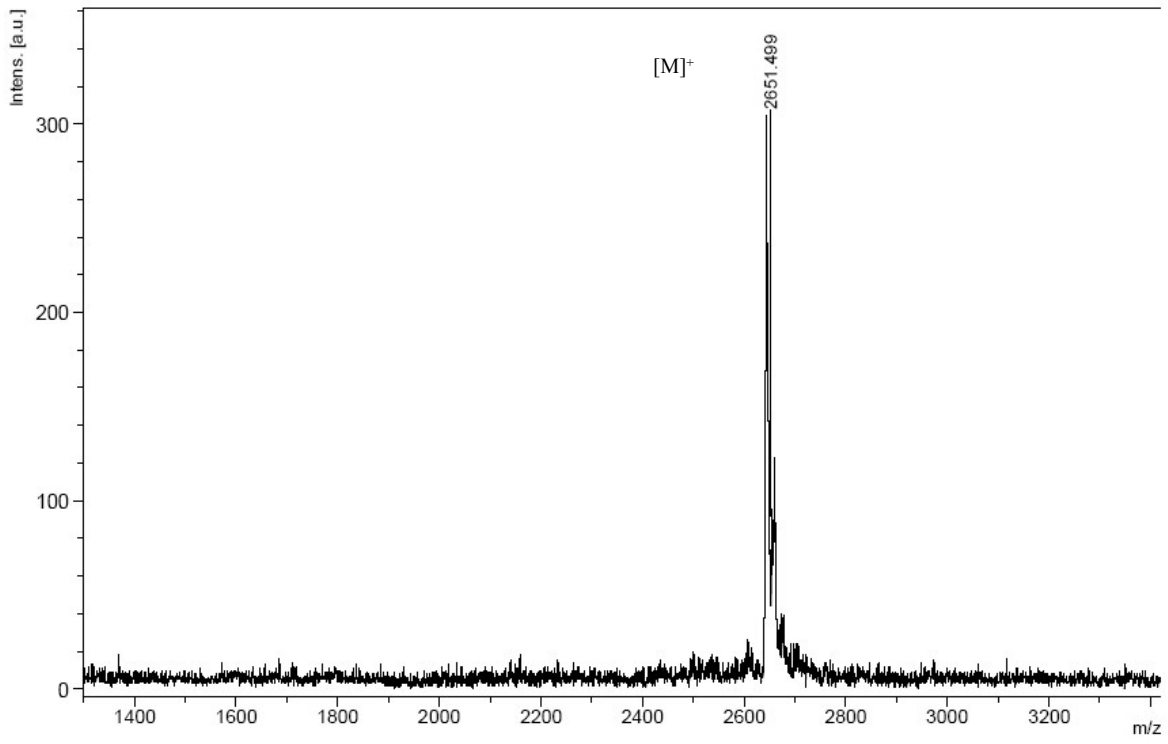

Figure S18. MALDI-TOF spectrum of compound **11b**

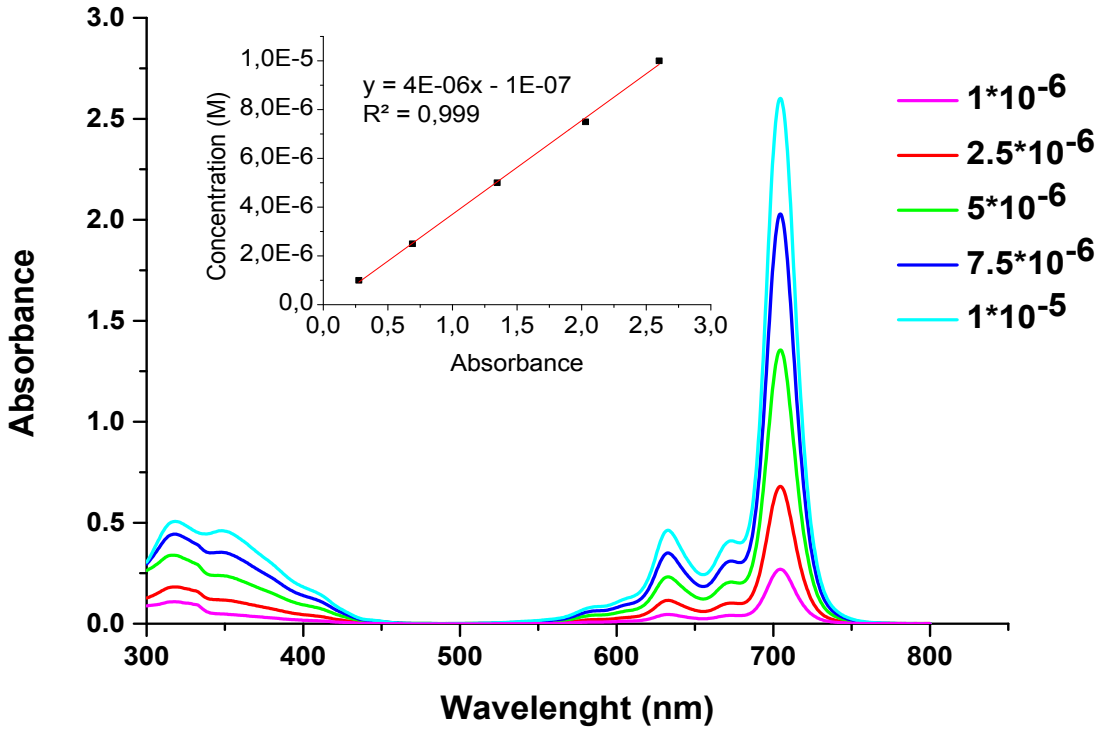

Fig. S19 Absorption spectra of THF solution of compound **10a** in different concentration

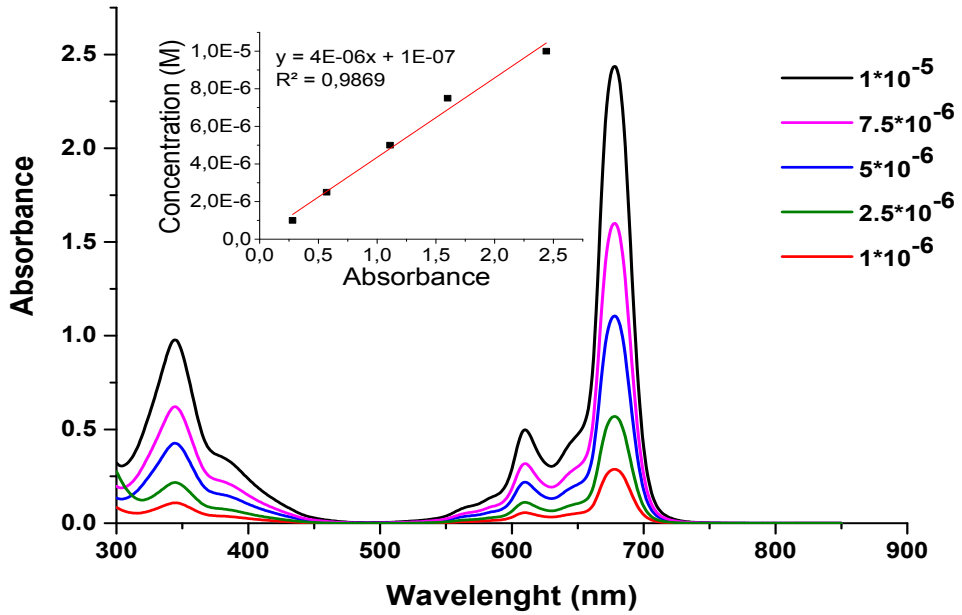

Fig. S20 Absorption spectra of THF solution of compound **11a** in different concentration

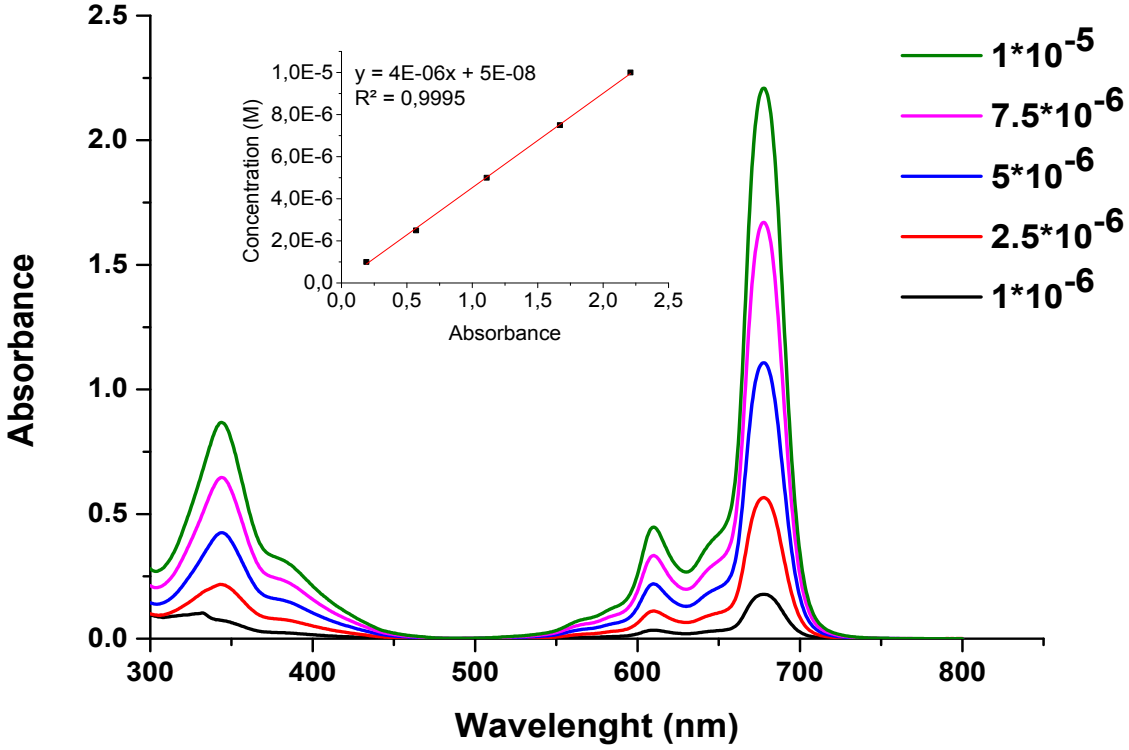

Fig. S21 Absorption spectra of THF solution of compound **11b** in different concentration

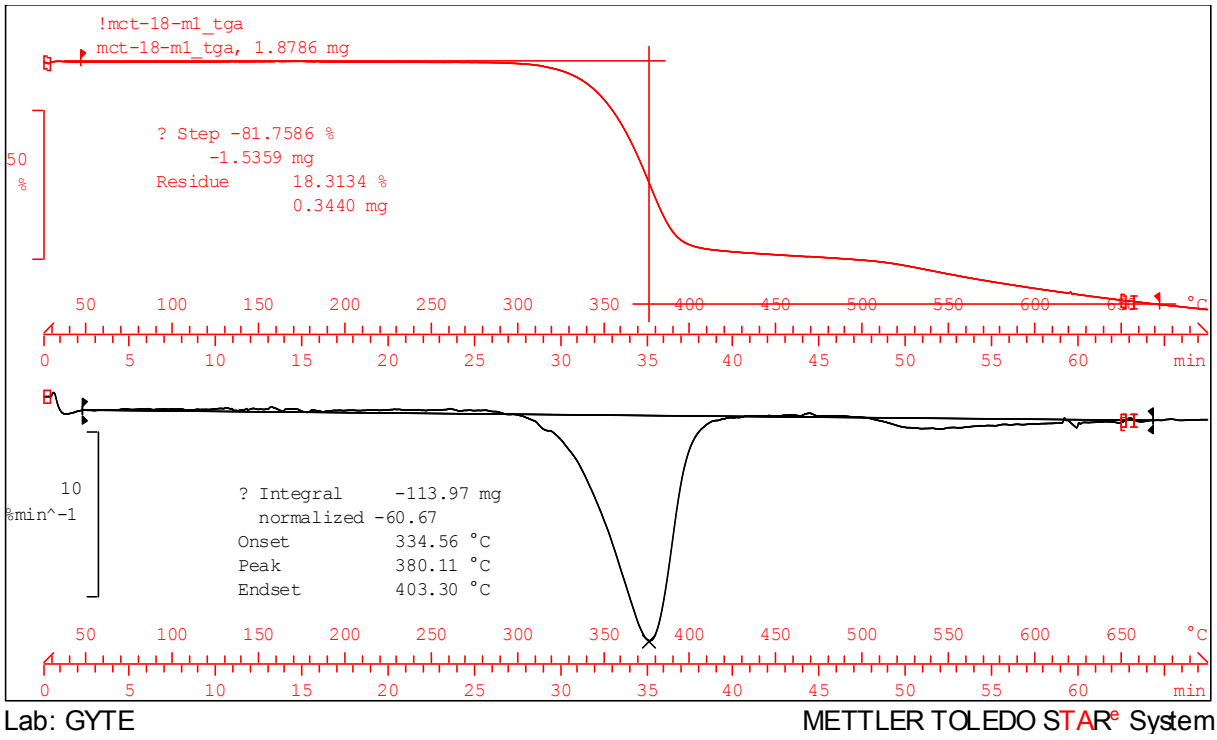

Fig. S22 TGA thermogram of **10a**.

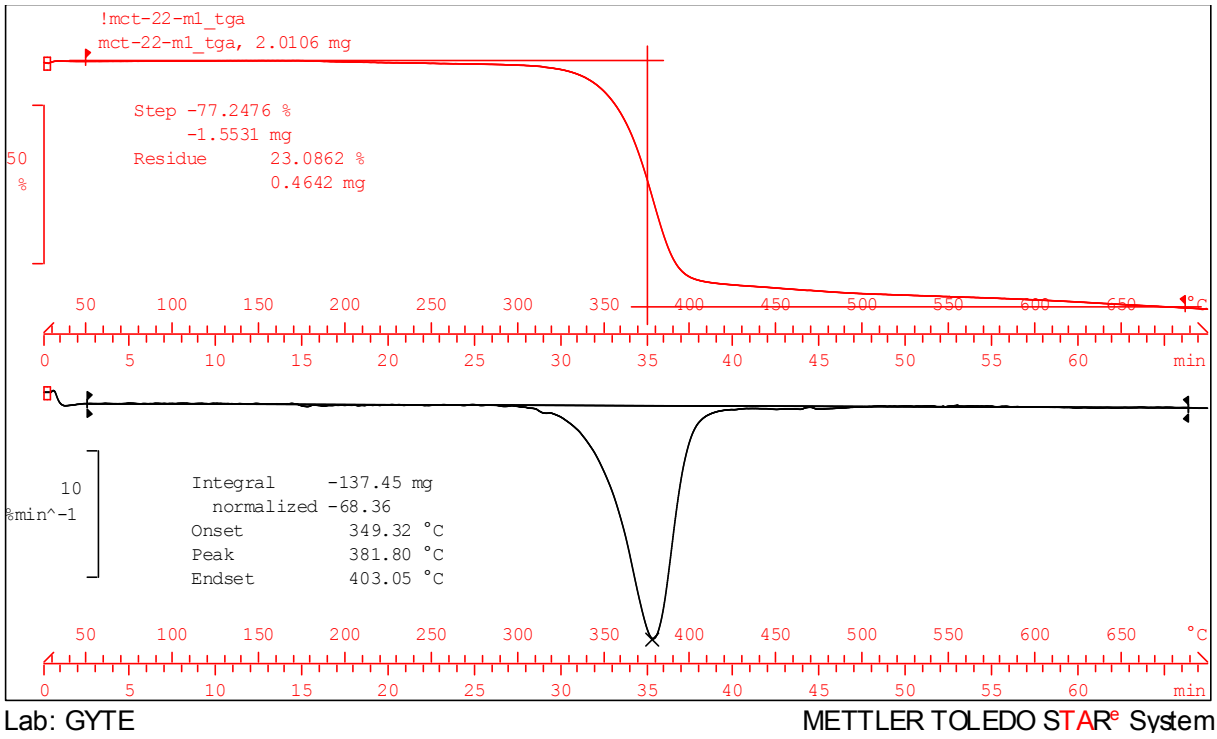

Fig. S23 TGA thermogram of **10b**.

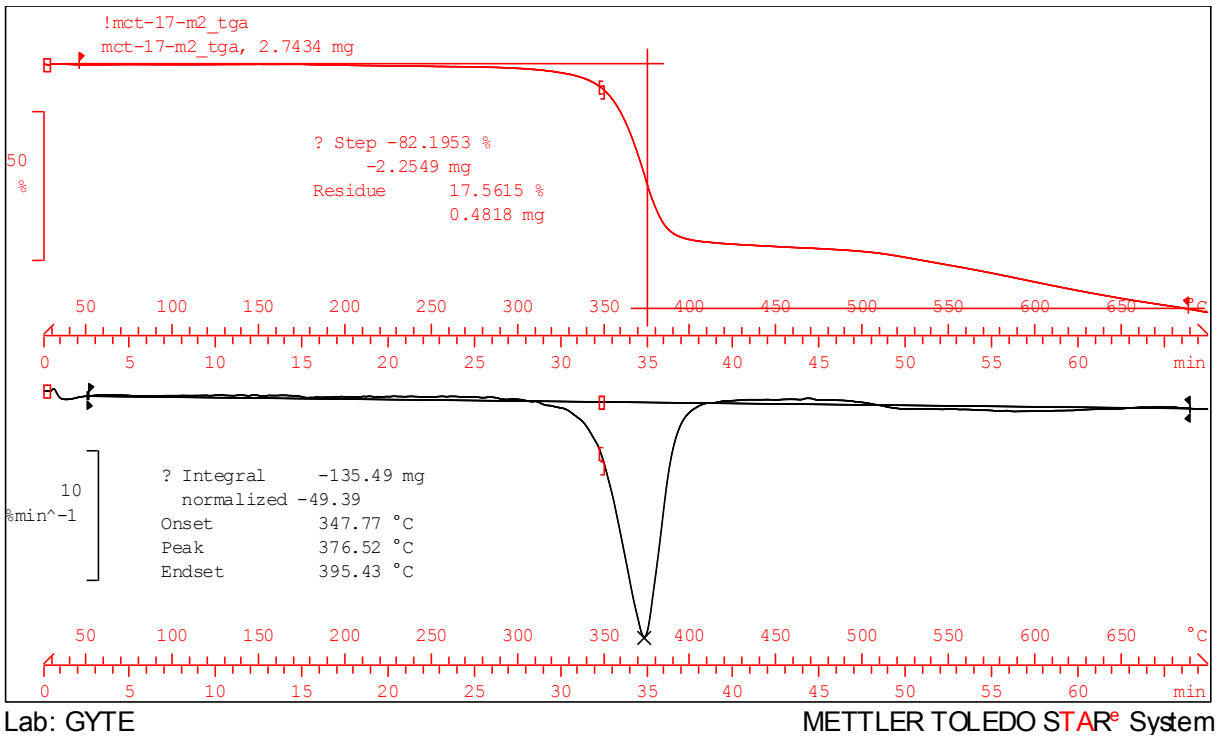

Fig. S24 TGA thermogram of **11a**.

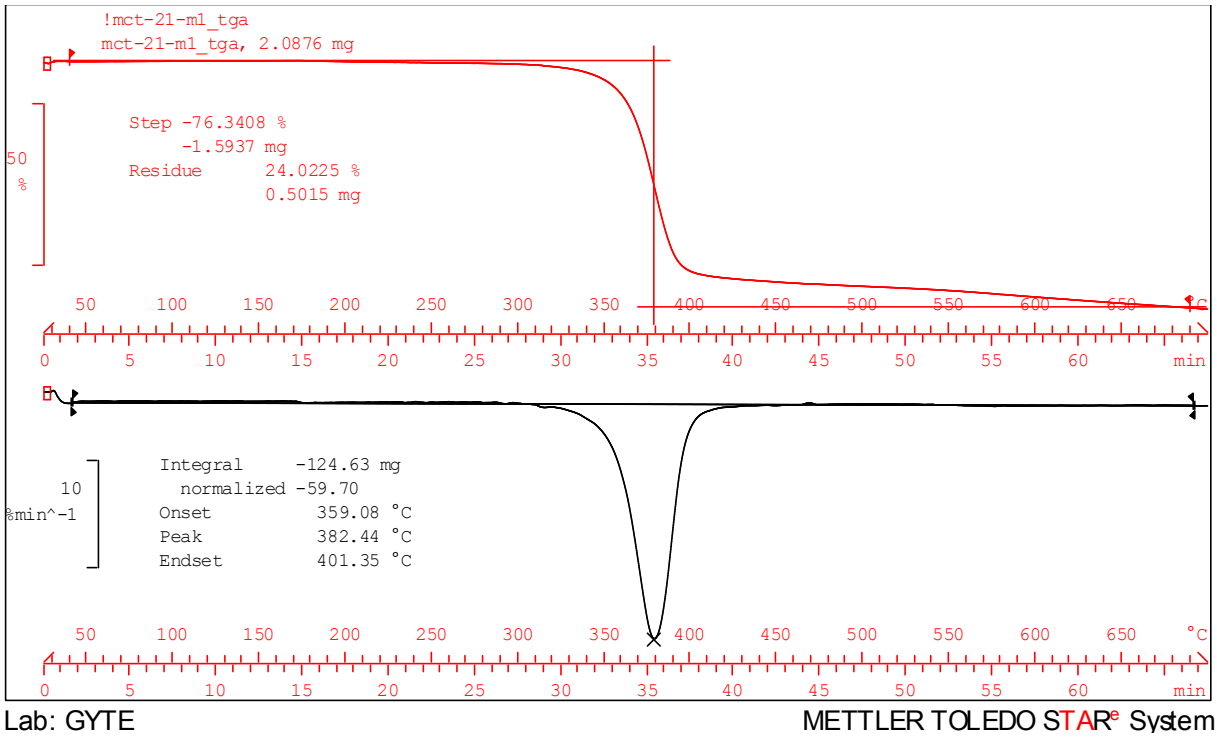

Fig. S25 TGA thermogram of **11b.**

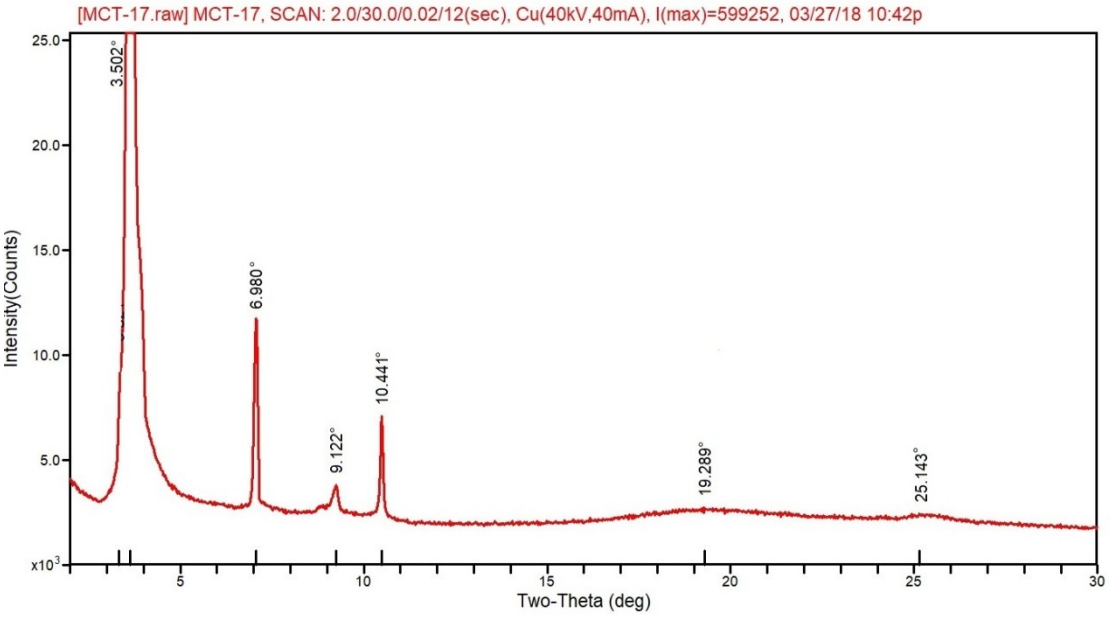

Fig. S26 XRD pattern of **11a.**

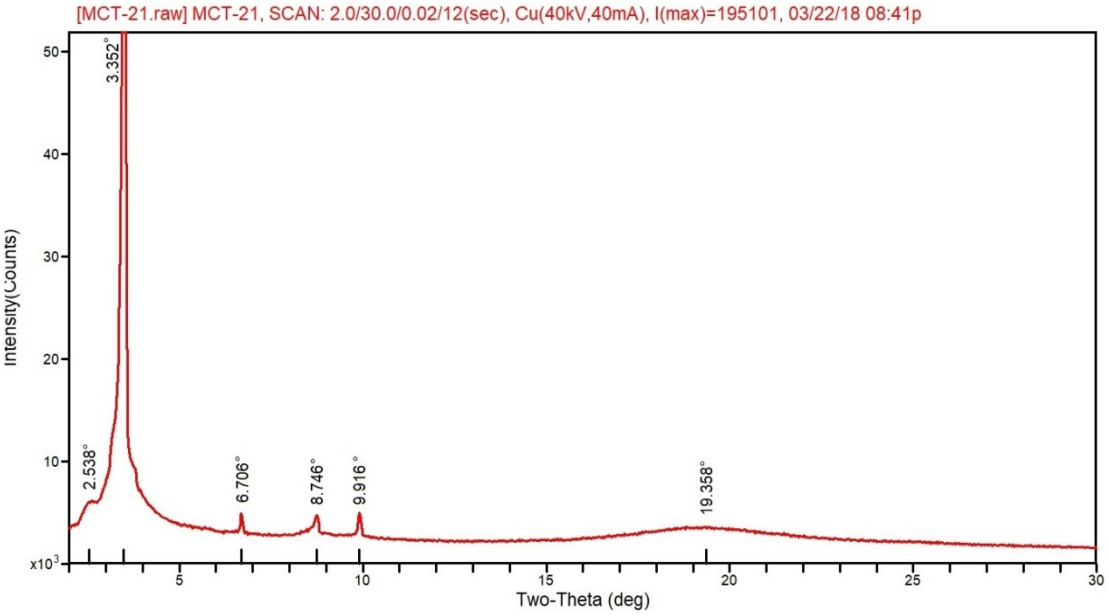

Fig. S27 XRD pattern of **11b.**