Supporting information

Cocrystals versus salts of fluorescein

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Table S1. Crystallographic data, details of data collection and structure refinement parameters for compounds **1**-**10**

Compound	**1**	**2**	**3**	**4**	**5**
Chemical formula	$C_{50}H_{32}N_2O_{10}$	$C_{52}H_{40}N_2O_{12}$	$C_{56}H_{46}N_2O_{12}$	$C_{32}H_{22}N_2O_5$	$C_{32}H_{24}N_2O_5$
M (g mol^{-1})	820.77	884.86	938.95	514.51	516.53
Temperature, (K)	293(2)	200(2)	173(2)	293(2)	200(2)
Wavelength, (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	*Monoclinic*	*Triclinic*	*Triclinic*	*Monoclinic*	*Monoclinic*
Space group	*P21/a*	*P-1*	*P-1*	*P21/c*	*P21/a*
a (Å)	7.9518(8)	7.7851(8)	7.7463(18)	16.1599(16)	13.109(2)
b (Å)	19.2982(16)	12.6149(12)	12.640(3)	12.1595(8)	12.5793(14)
c (Å)	12.9588(11)	12.7770(13)	12.950(5)	13.0564(8)	15.8101(14)
α (º)	90	116.587(8)	108.75(2)	90	90
β (º)	95.196(8)	107.300(8)	100.06(3)	101.511(7)	102.130(13)
γ (º)	90	90.681(8)	90.911(18)	90	90
V (Å^3)	1980.4(3)	1055.8(2)	1178.7(6)	2513.9(3)	2548.9(5)
Z	2	1	1	4	4
D_c (g cm^{-3})	1.376	1.392	1.323	1.359	1.346
μ (mm^{-1})	0.097	0.100	0.093	0.093	0.092
F(000)	852	462	492	1072	1080
Goodness-of-fit on F^2	0.825	0.927	0.794	1.061	0.972
Final R_1, wR_2 [I>2σ(I)]	0.0403, 0.0909	0.0526, 0.0921	0.0444, 0.0786	0.0937, 0.1929	0.0715, 0.1462
R_1, wR_2 (all data)	0.0883, 0.1051	0.1281, 0.1162	0.1252, 0.0961	0.1943, 0.2386	0.1863, 0.2029

Compound	**6**	**7**	**8**	**9**	**10**
Chemical formula	$C_{25}H_{22}N_2O_7$	$C_{25}H_{18}N_2O_5$	$C_{26}H_{32}N_2O_8$	$C_{47}H_{45}N_2O_{12.5}$	$C_{98}H_{98}N_6O_{24}$
M (g mol^{-1})	462.44	426.41	500.53	837.85	1743.82
Temperature, (K)	200(2)	293(2)	173(2)	293(2)	293(2)
Wavelength, (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	*Triclinic*	*Monoclinic*	*Triclinic*	*Triclinic*	*Triclinic*
Space group	*P-1*	*C2/c*	*P-1*	*P-1*	*P-1*
a (Å)	7.9208(13)	26.783(4)	8.0595(6)	11.2955(3)	11.8141(12)
b (Å)	11.1684(19)	19.468(3)	11.4011(10)	13.9824(3)	13.8225(13)
c (Å)	14.678(3)	7.7431(13)	13.5000(10)	14.1629(3)	14.5549(17)
α (º)	111.235(14)	90	87.086(6)	97.069(2)	98.060(8)
β (º)	92.364(14)	94.033(13)	74.482(6)	108.163(2)	103.933(9)
γ (º)	109.493(13)	90	80.885(6)	102.315(2)	109.797(7)
V (Å^3)	1121.3(4)	4027.5(11)	1180.12(17)	2032.75(9)	2105.6(4)
Z	2	8	2	2	1
D_c (g cm^{-3})	1.370	1.406	1.409	1.369	1.375
μ (mm^{-1})	0.101	0.099	0.105	0.100	0.099
F(000)	484	1776	532	882	920
Goodness-of-fit on F^2	1.007	0.891	0.987	1.103	0.808
Final R_1, wR_2 [I>2σ(I)]	0.0701, 0.0974	0.0780, 0.1766	0.0475, 0.1133	0.0438, 0.1192	0.0605, 0.1317
R_1, wR_2 (all data)	0.1908, 0.1329	0.2427, 0.2557	0.0858, 0.1265	0.0536, 0.1257	0.1846, 0.1713

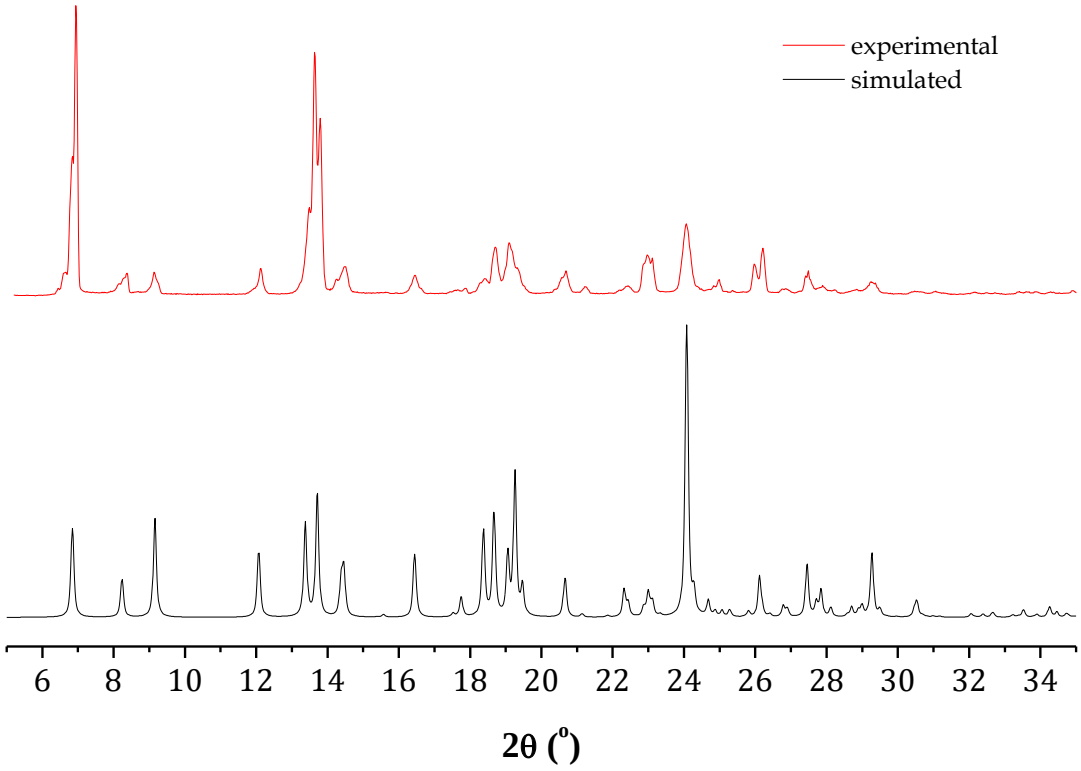

Figure S1. Measured (red) and calculated (black) powder X-ray diffraction patterns of **1**.

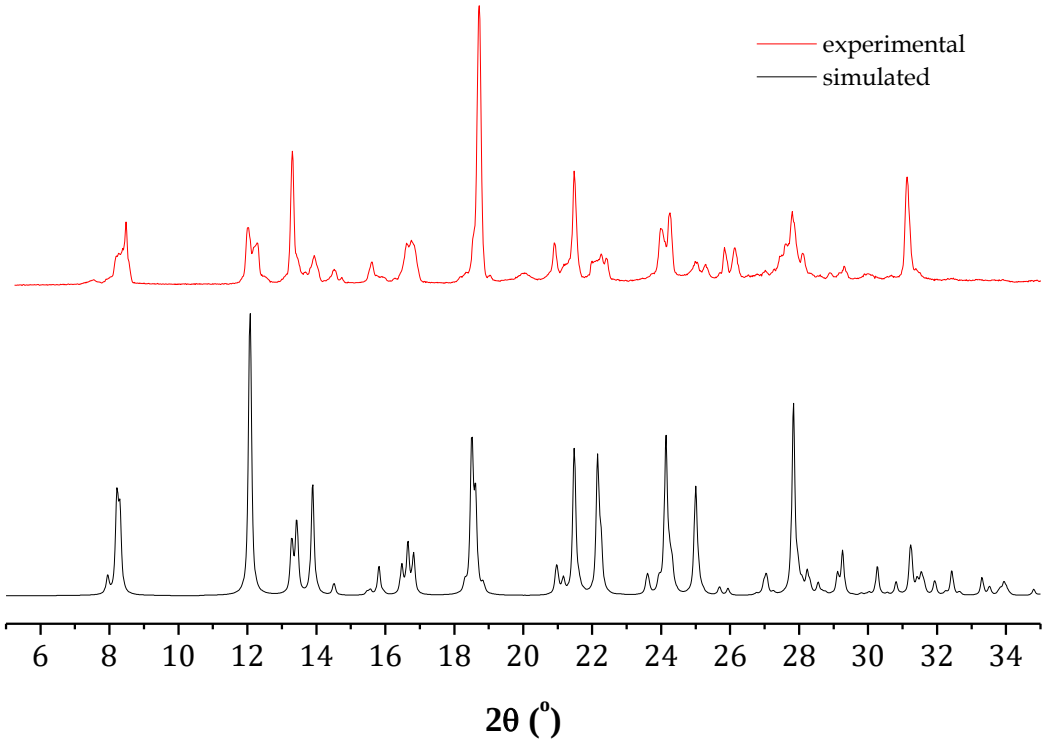

Figure S2. Measured (red) and calculated (black) powder X-ray diffraction patterns of **2**.

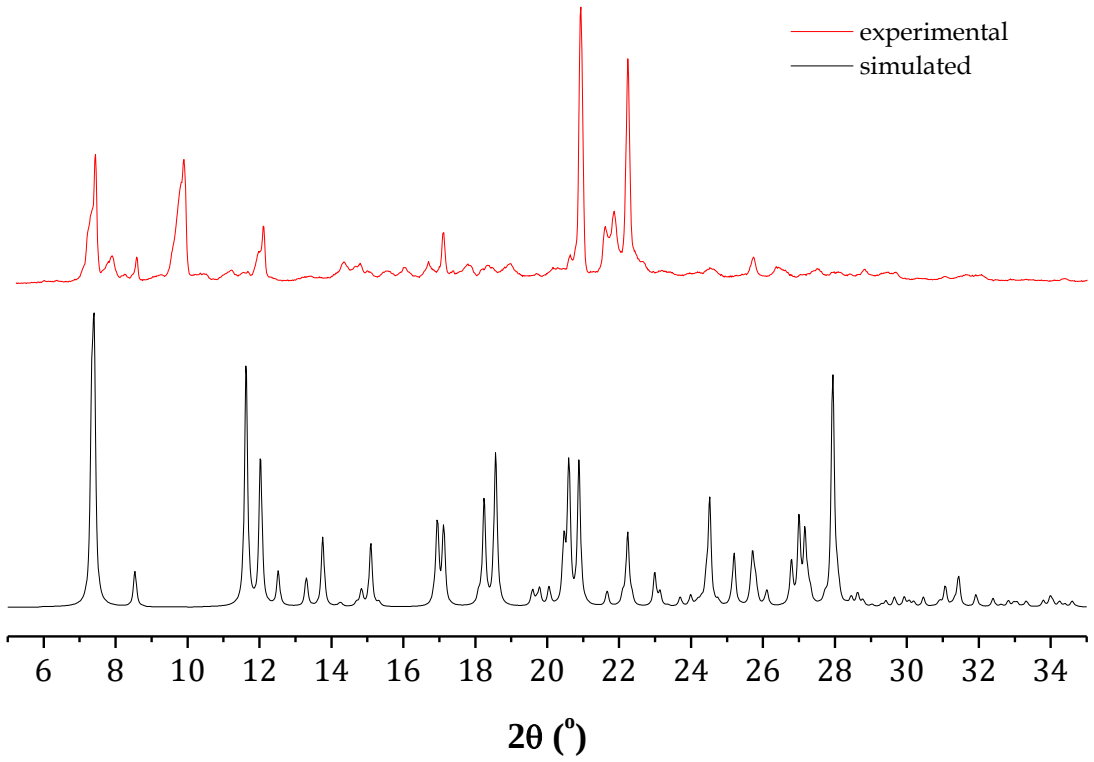

Figure S3. Measured (red) and calculated (black) powder X-ray diffraction patterns of **3**.

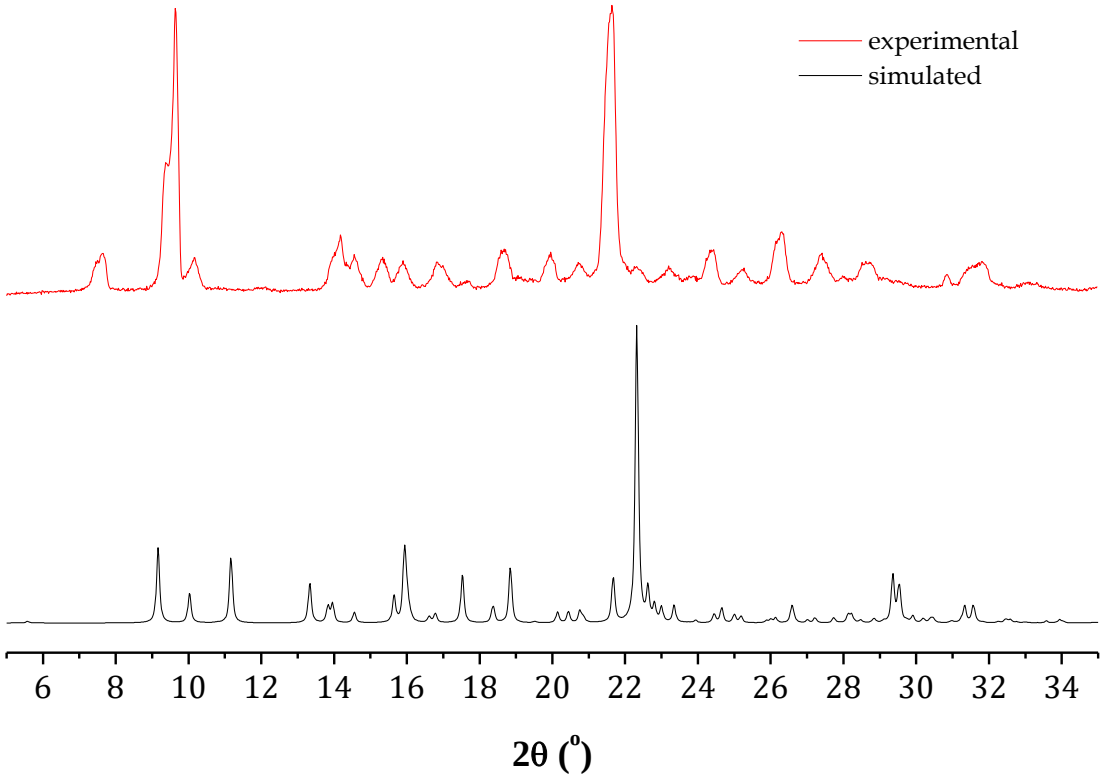

Figure S4. Measured (red) and calculated (black) powder X-ray diffraction patterns of **4**.

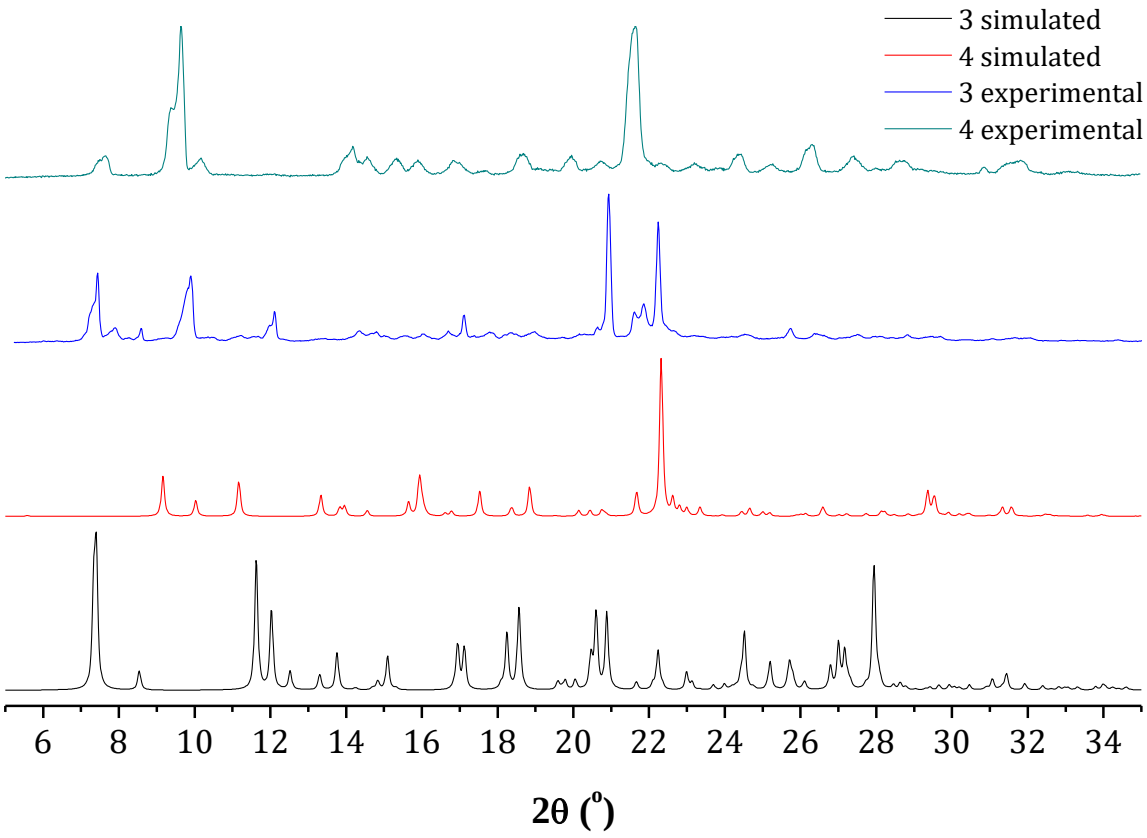

Figure S5. Comparison between powder X-ray diffraction patterns of **3** and **4**.

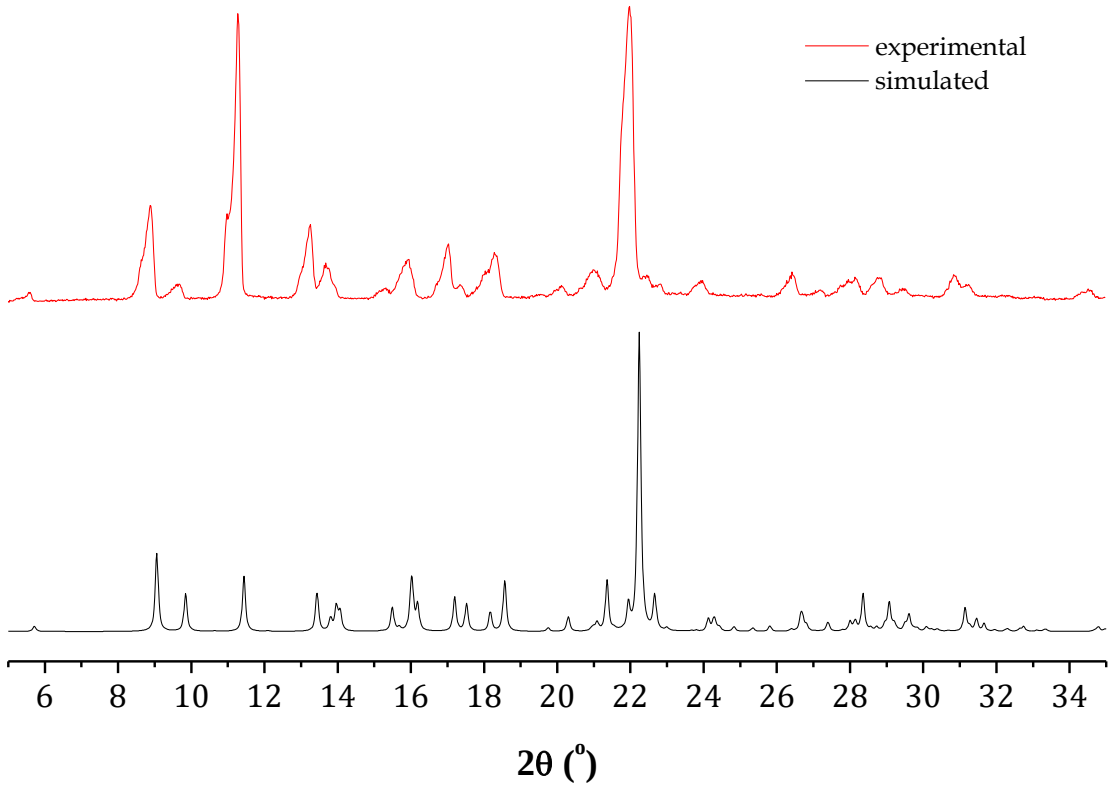

Figure S6. Measured (red) and calculated (black) powder X-ray diffraction patterns of **5**.

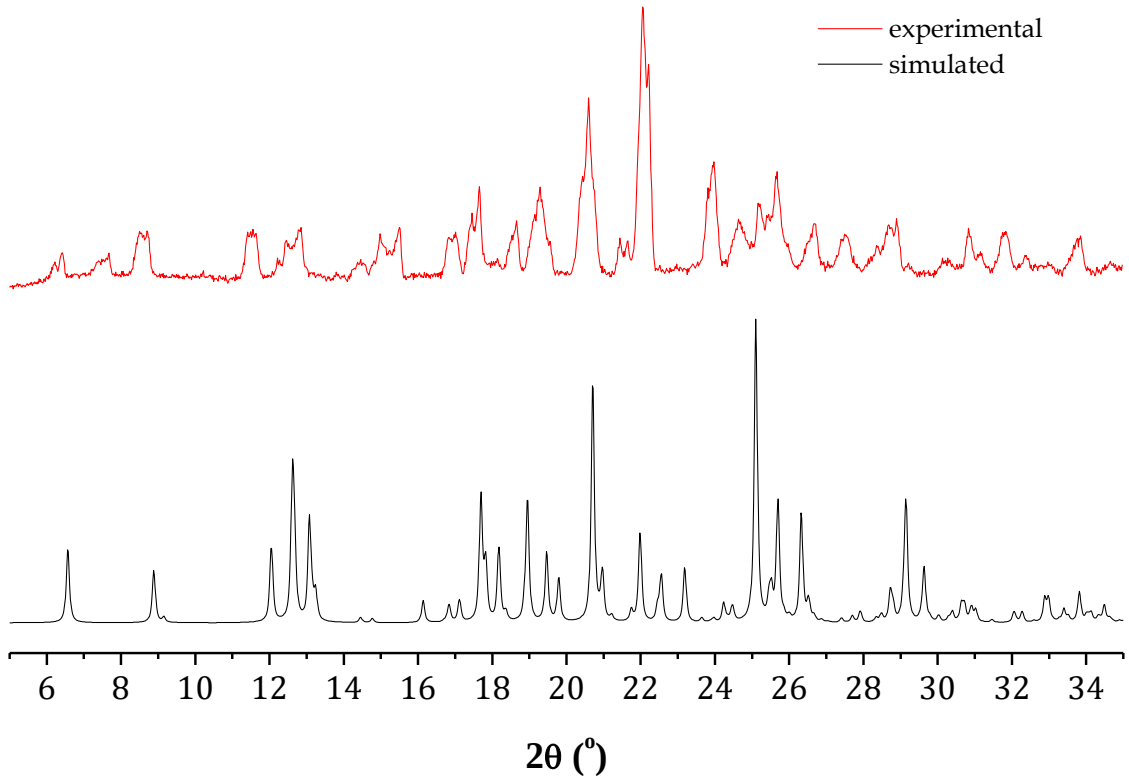

Figure S7. Measured (red) and calculated (black) powder X-ray diffraction patterns of **6**.

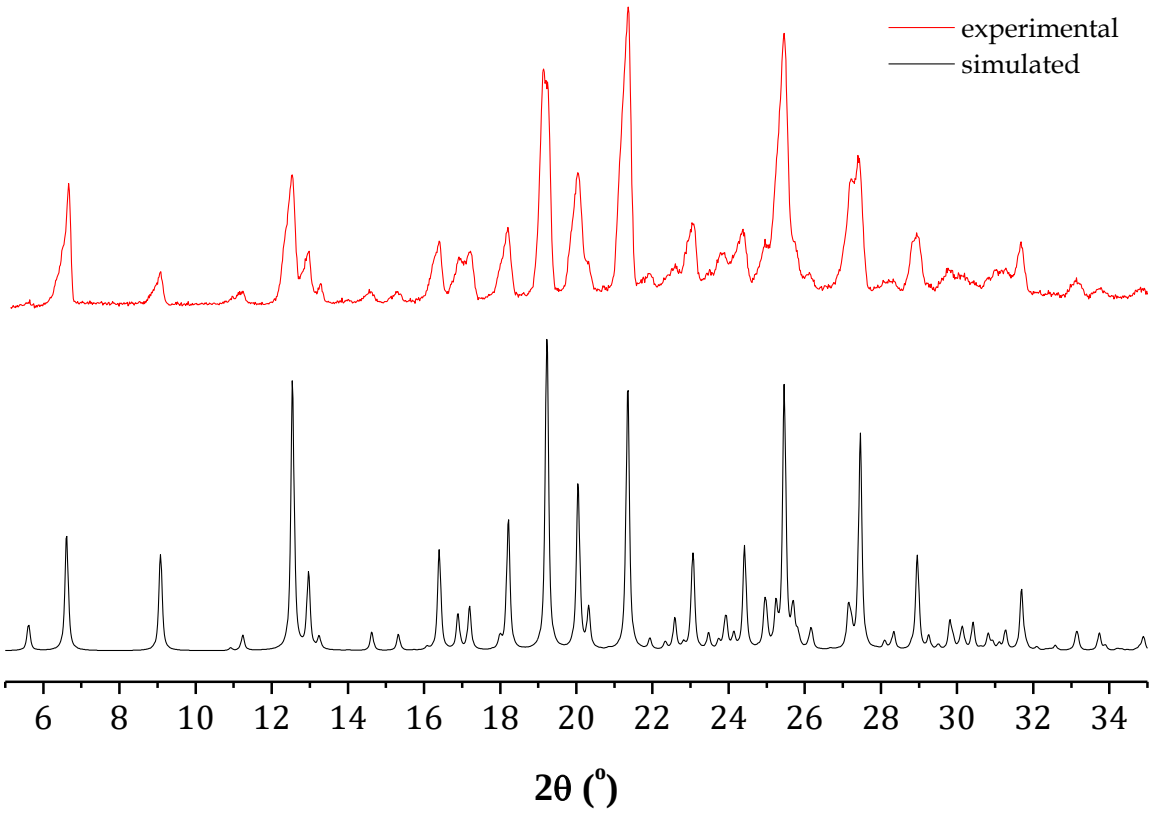

Figure S8. Measured (red) and calculated (black) powder X-ray diffraction patterns of **7**.

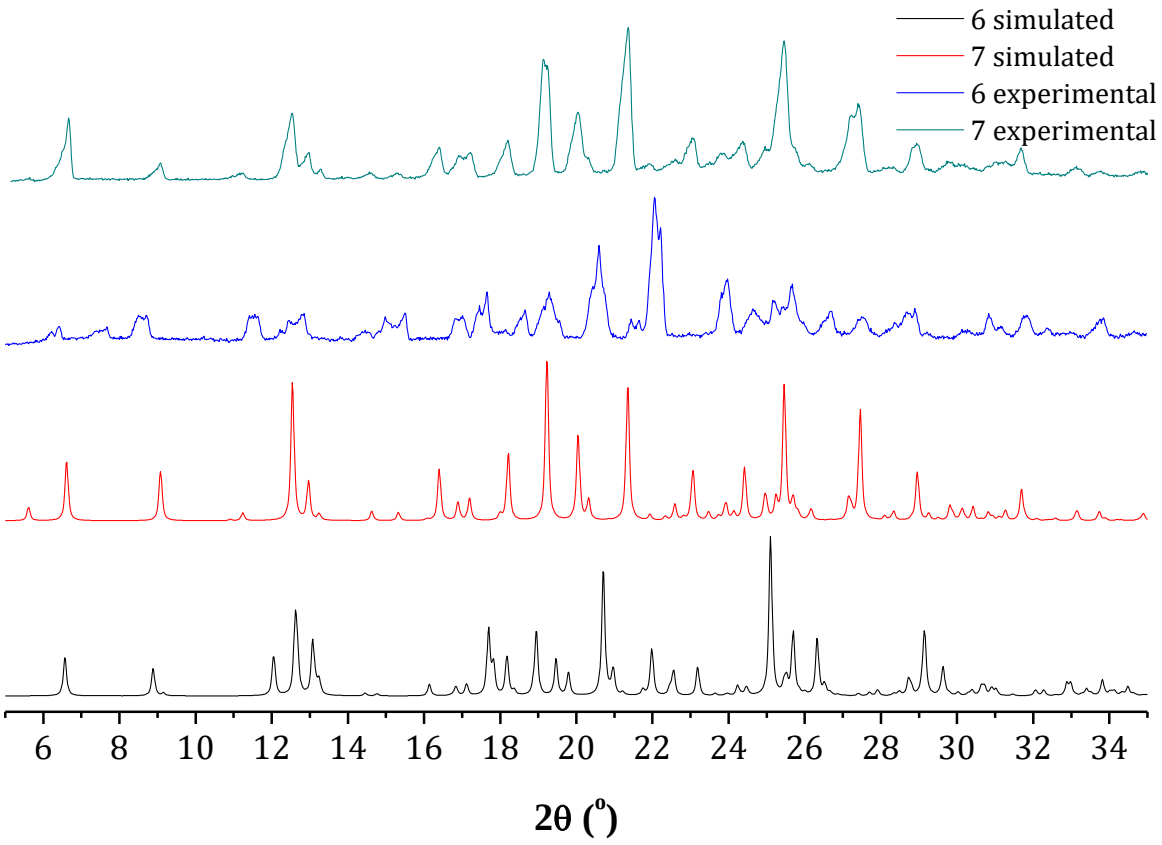

Figure S9. Comparison between powder X-ray diffraction patterns of **6** and **7**.

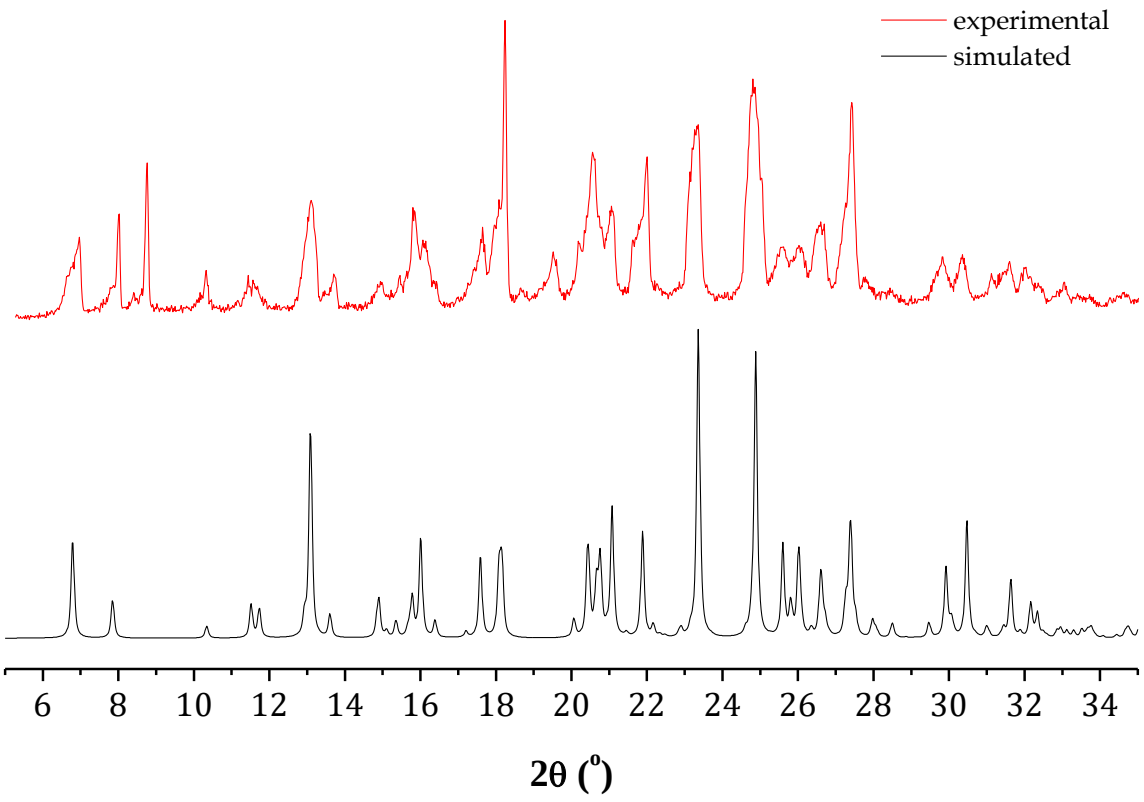

Figure S10. Measured (red) and calculated (black) powder X-ray diffraction patterns of **8**.

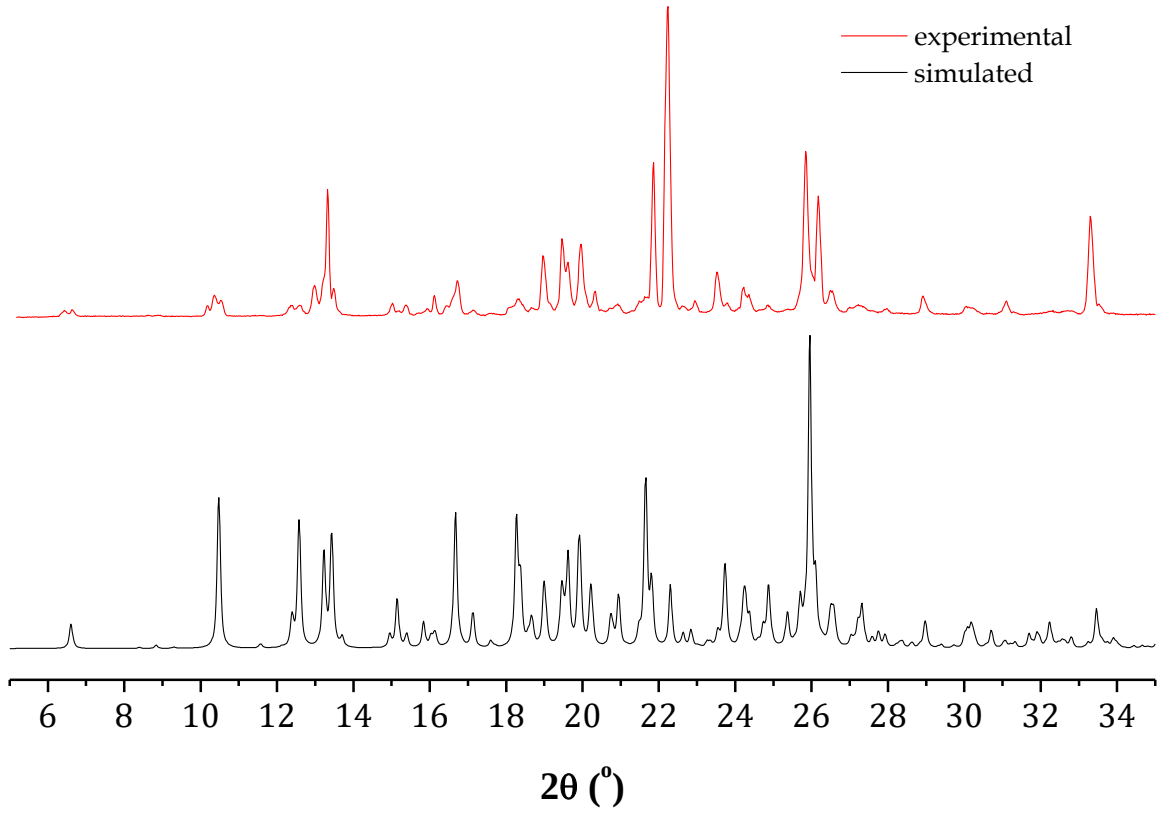

Figure S11. Measured (red) and calculated (black) powder X-ray diffraction patterns of **9**.

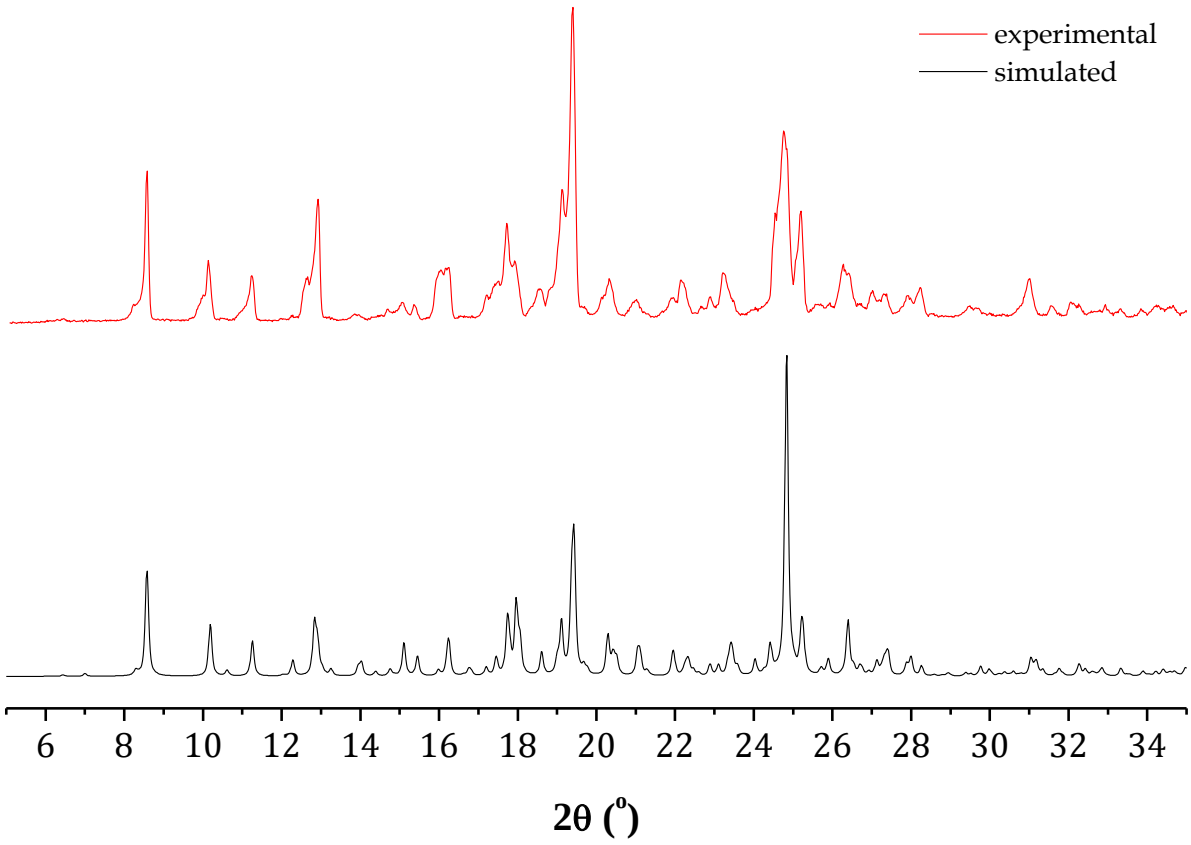

Figure S12. Measured (red) and calculated (black) powder X-ray diffraction patterns of **10**.

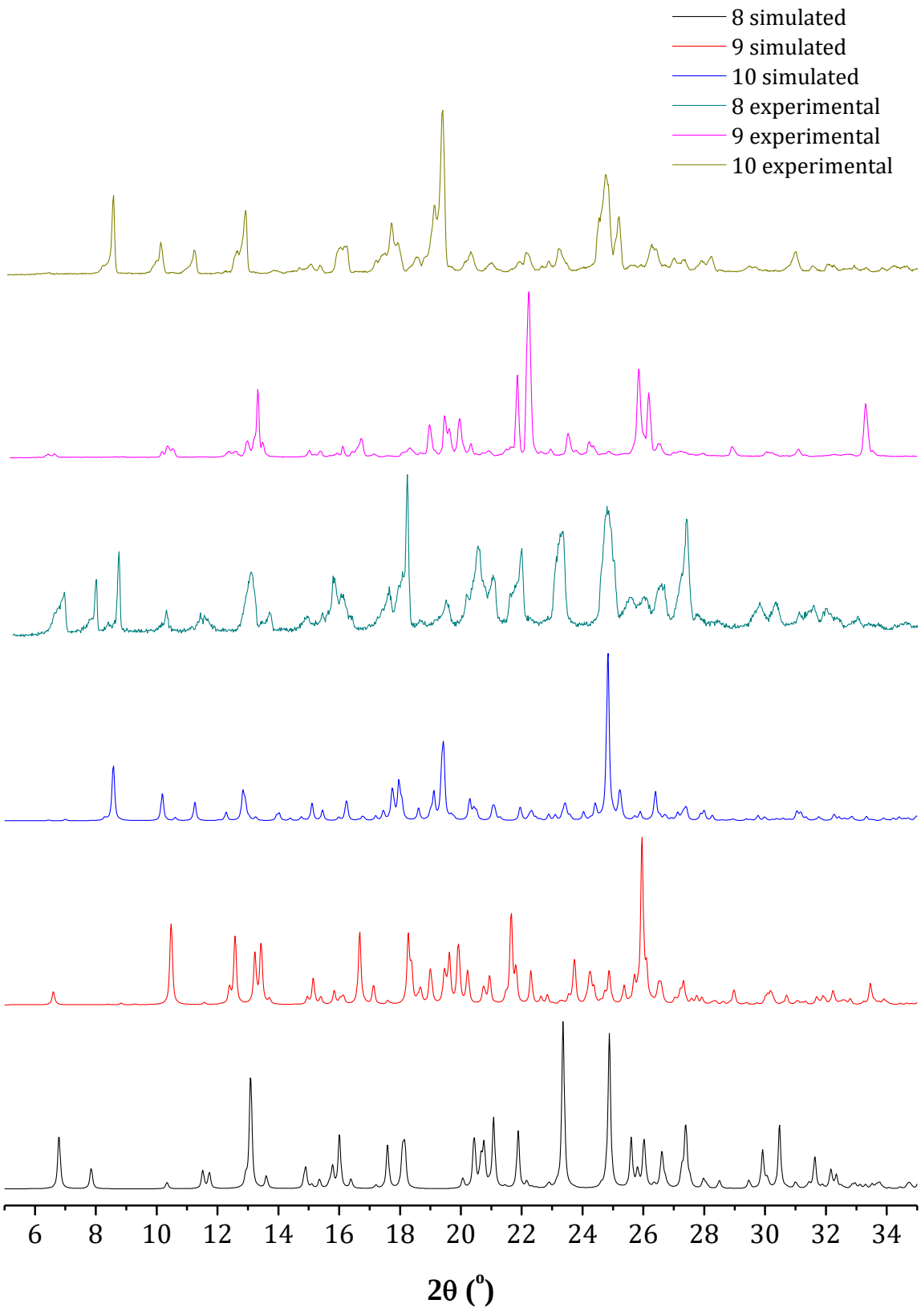

Figure S13. Comparison between powder X-ray diffraction patterns of **8**, **9** and **10**.