Supporting Information

Table S1 Selected bond lengths (Å) for **1-3**.

	1	**2**	**3**
P1-O1	1.574(1)	1.578(2)	1.561(4)
P1-O2	1.558(1)	1.566(3)	1.546(4)
P1-O3	1.457(1)	1.456(3)	1.502(4)
C1-P1	1.829(2)	1.806(3)	1.770(6)
C1-C2	1.521(3)	1.517(4)	1.557(7)
O2-C18	1.455(3)	1.440(5)	1.466(7)
O1-C16	1.446(3)	1.447(4)	
Br1-C9		1.902(3)	1.908(6)
Br2-C18			1.930(6)
C1-O4	1.400(3)		

Table S2 Fluorescence lifetimes of **1-3** in CH_2Cl_2 solution and in solid state.

In solution	**1**			**2**			**3**		
Emission (nm)	399	420	445	412	434	458	413	436	460
Lifetime (ns)	2.4	2.2	2.2	0.78	0.68	0.72	0.72	0.71	0.71
In solid state	**1**			**2**			**3**		
Emission (nm)	438		456	476		496	449	475	483
Lifetime (ns, τ_1)	1.7		1.4	0.86		0.94	0.53	0.65	0.73
Lifetime (ns, τ_2)	4.6		4.6	2.4		3.2	3.3	3.8	3.8

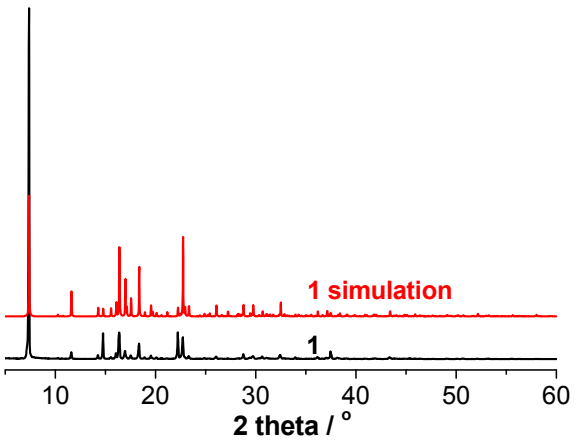

Fig. S1 Experimental and simulated XRD patterns of **1**.

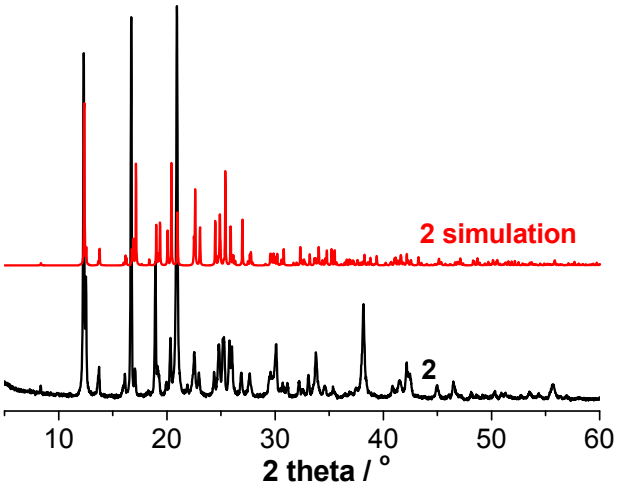

Fig. S2 Experimental and simulated XRD patterns of **2**.

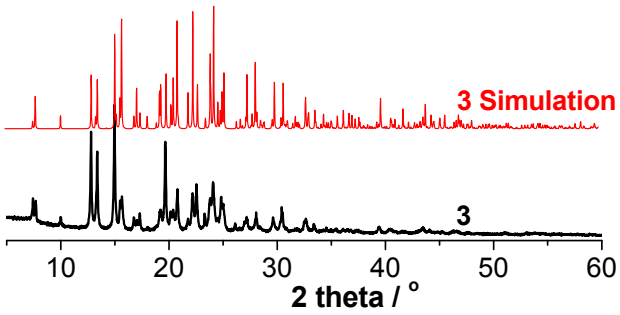

Fig. S3 Experimental and simulated XRD patterns of **3**.

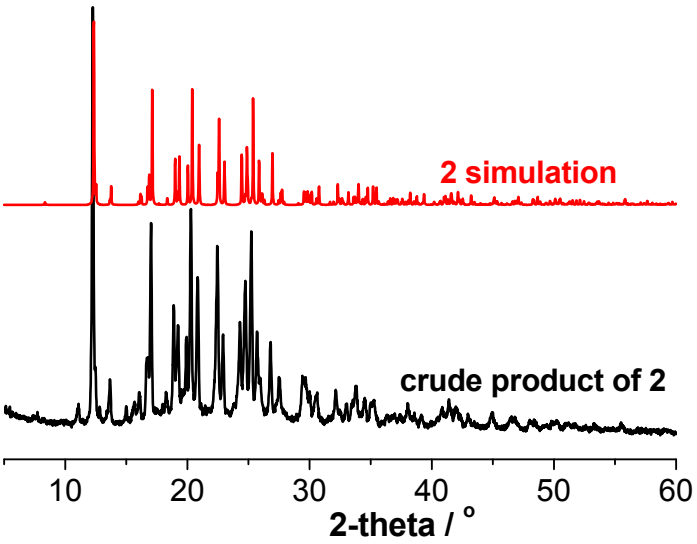

Fig. S4 The XRD pattern for the crude product of **2** obtained from the dry CH_3CN solution, and the simulated XRD pattern.

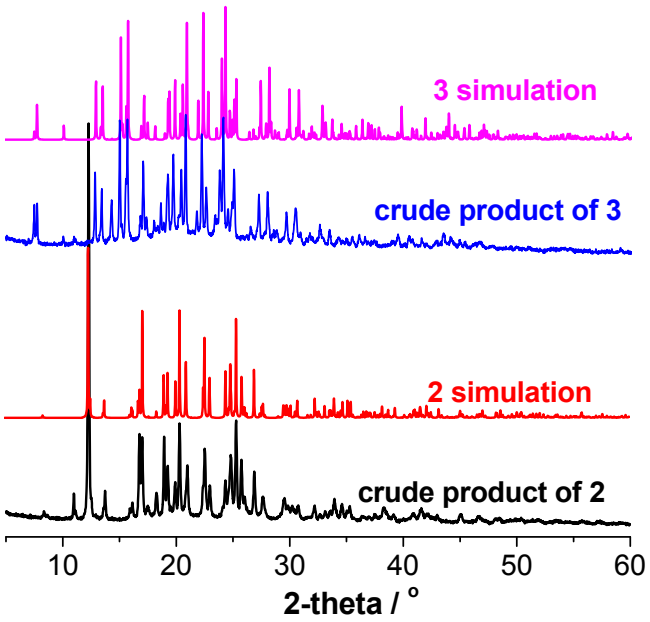

Fig. S5 The XRD patterns for the crude products of **2** and **3** obtained from the isolation with High-Preparative Liquid Chromatography, and their simulated XRD patterns.

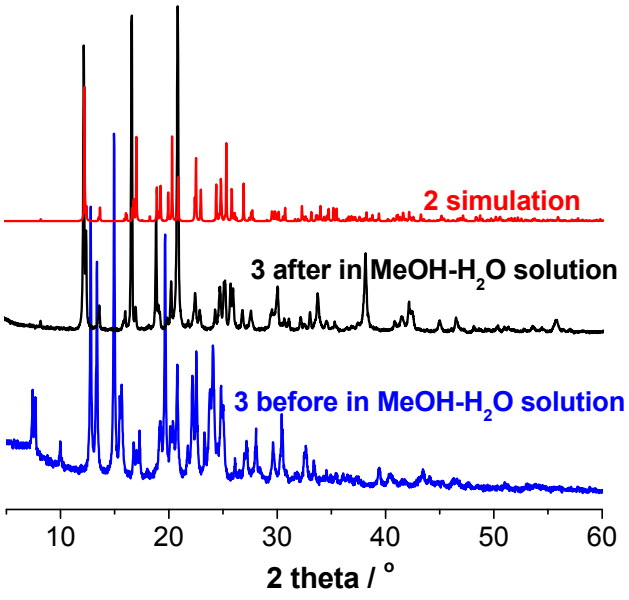

Fig. S6 The XRD patterns of **3** before and after staying in CH_3OH-H_2O solution, and the simulated XRD pattern of **2**.

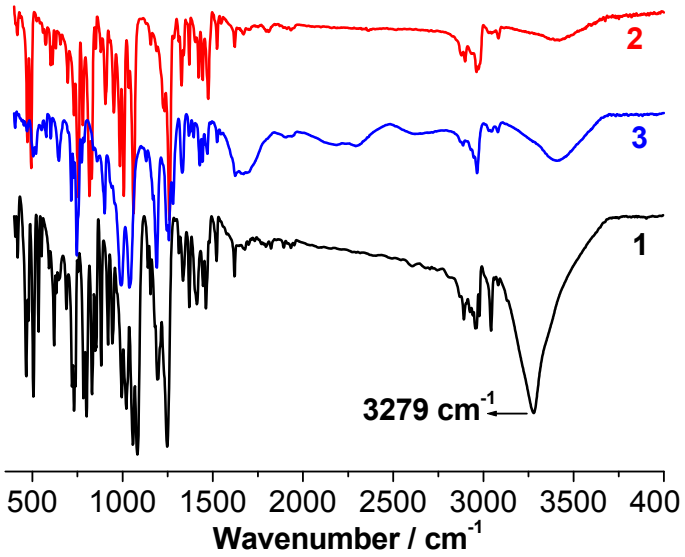

Fig. S7 IR spectra of **1** - **3**.

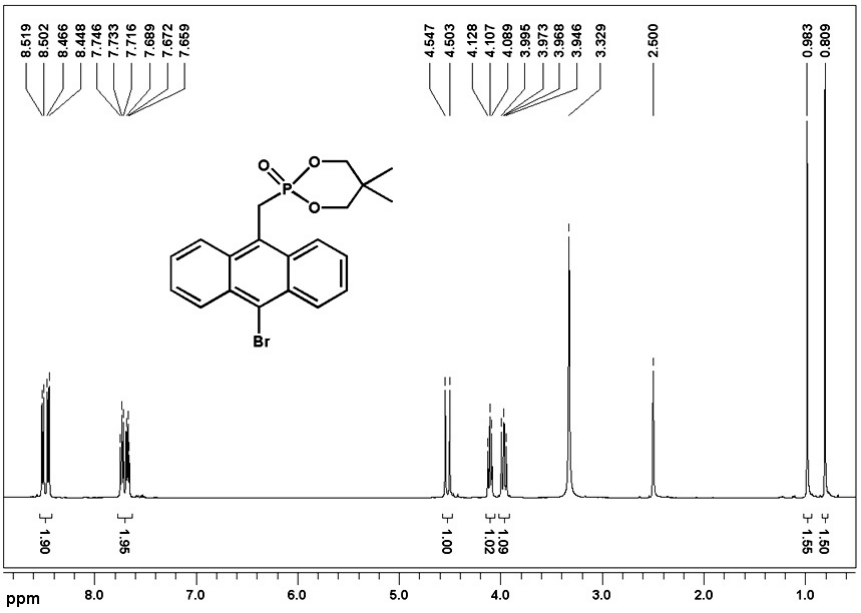

Fig. S8 ^{1}H NMR spectrum of **2** (500 MHz, DMSO-d_6).

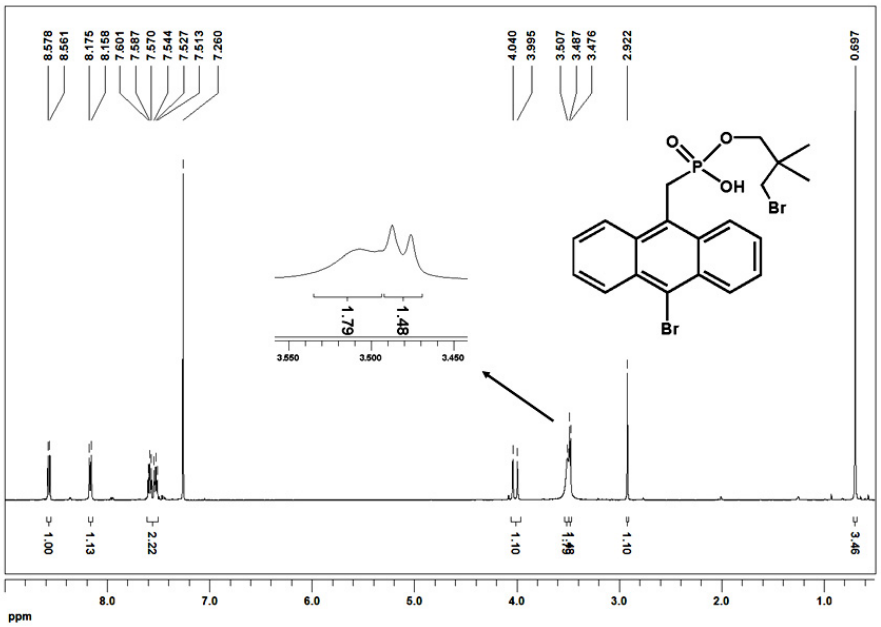

Fig. S9 ^{1}H NMR spectrum of **3** (500 MHz, $CDCl_3$).