Supporting Information

Substituted Benzoxazole and Catechol Cocrystals as an Adsorbent for CO_2 Capture: Synthesis and Mechanistic Studies

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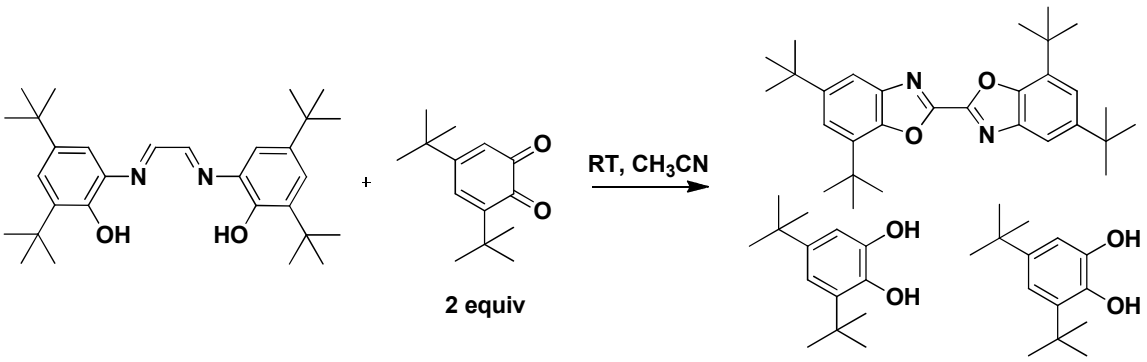
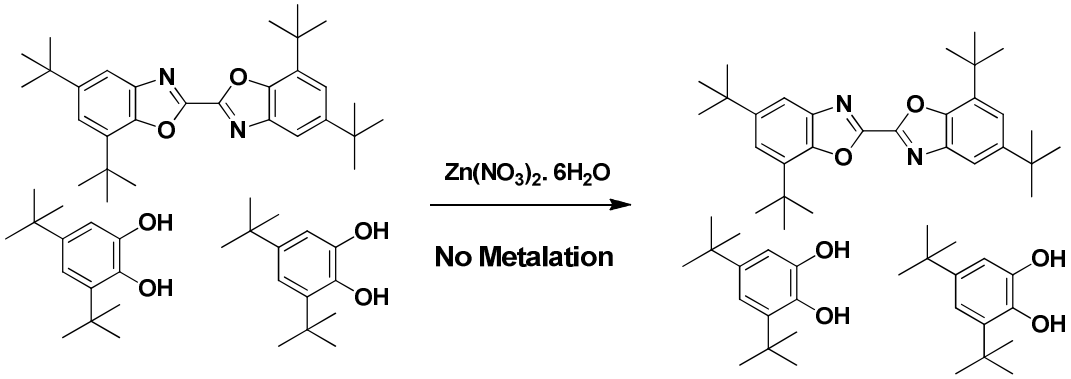
Contents



Scheme S1: Synthesis of **2**



Note that the presence of hydrogen bonds between the substituted benzoxazole and catechol in **2** avoided the metalation of benzoxazole nitrogen atoms of **2** with a metal precursor, when $Zn(NO_3)_2 \cdot 6H_2O$ and **2** at a 1:1 ratio were combined in MeOH at room temperature for 12 h.

Scheme S2: Metalation of **2** with $Zn(NO_3)_2.6H_2O$

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

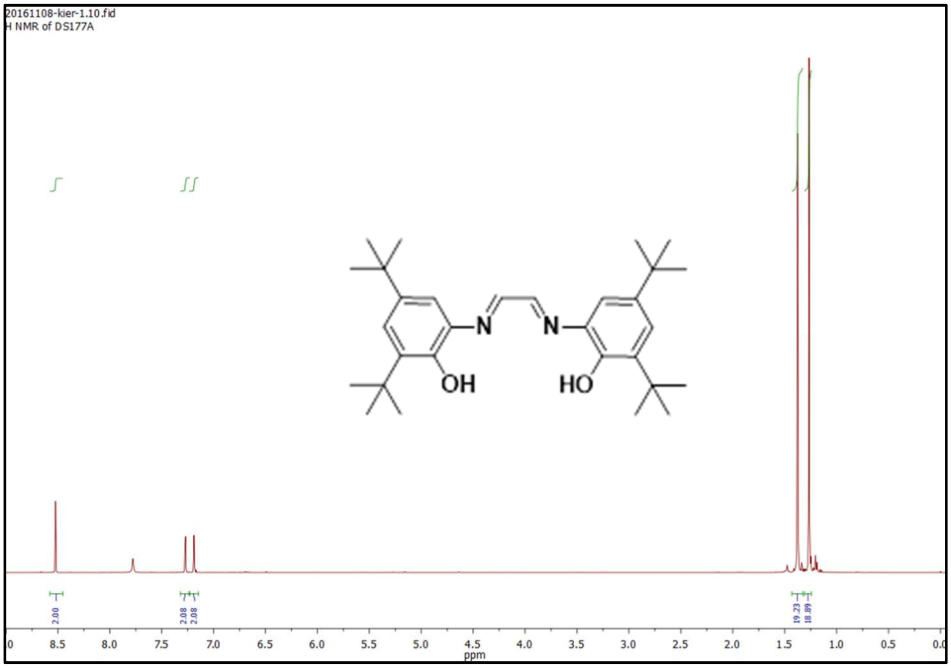


Figure S1A. ^{13}C NMR spectrum of **1**

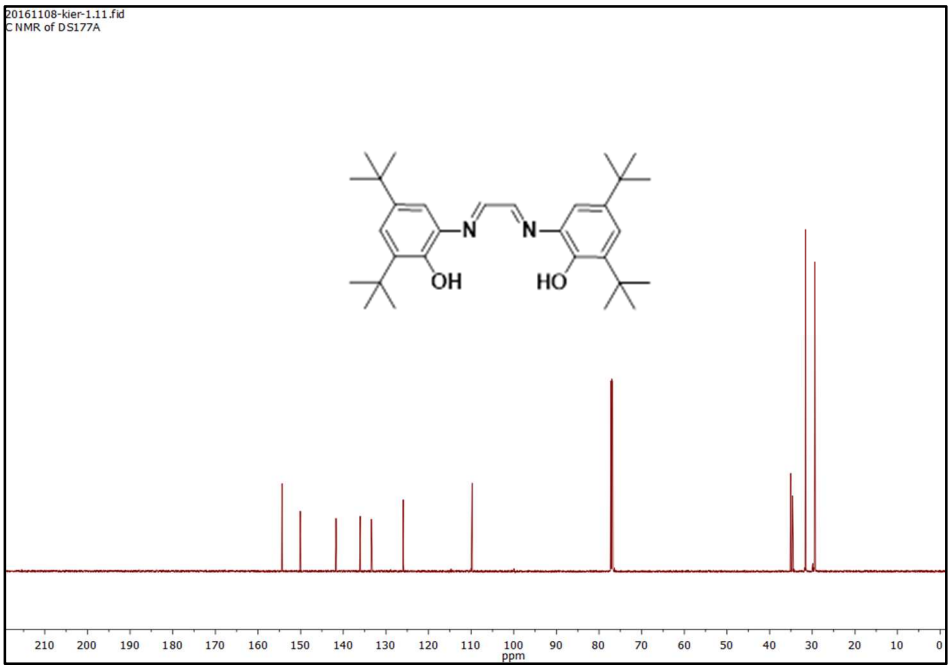


Figure S2. ^{1}H NMR spectrum of **2**

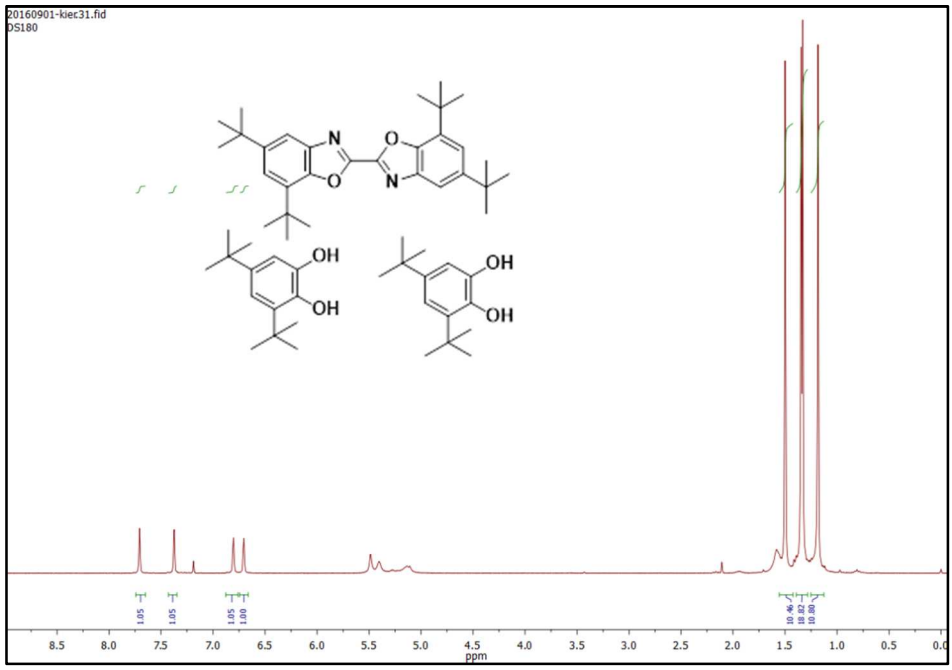


Figure S2A. ^{13}C NMR spectrum of **2**

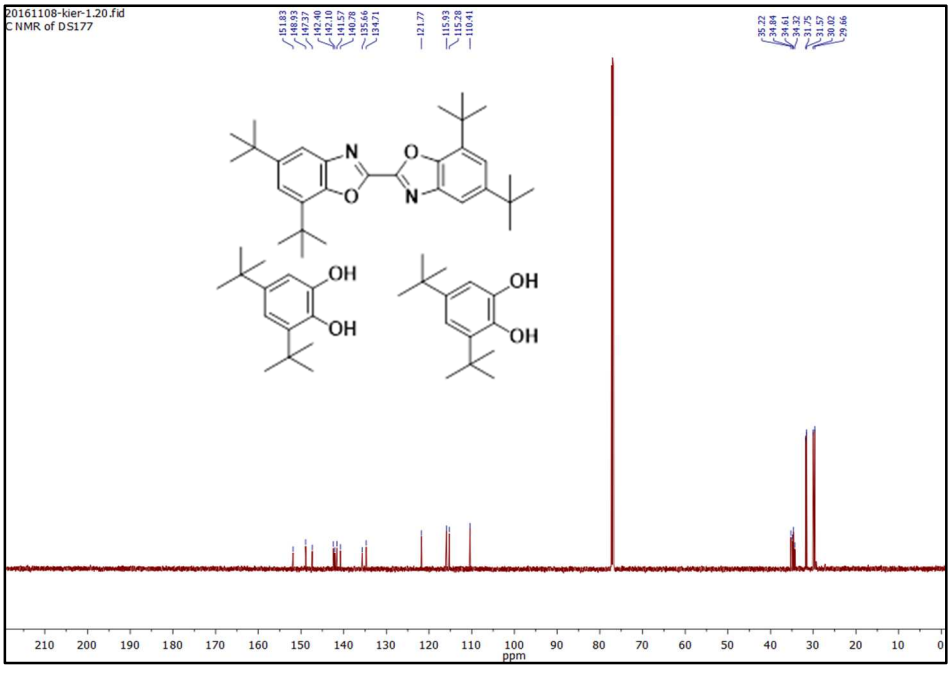


Figure S3. FT-IR spectra of **1**(imine) and **2**

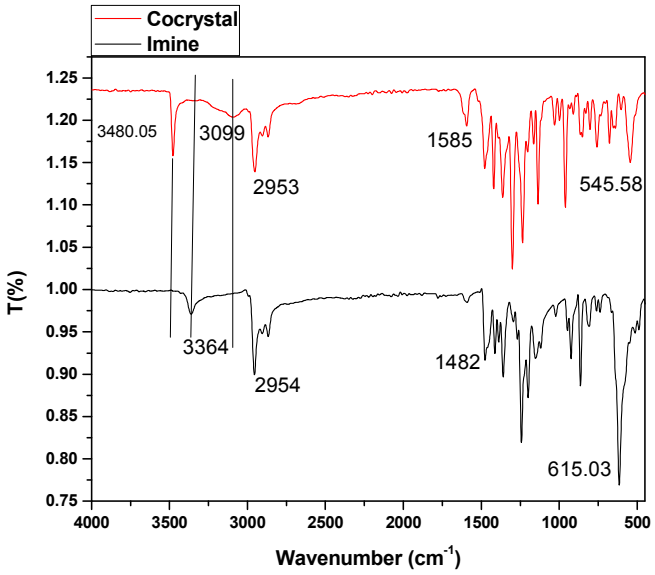


Figure S4. N…H-O and O-H..O hydrogen bonds form parallel chain along a-axis in **2**

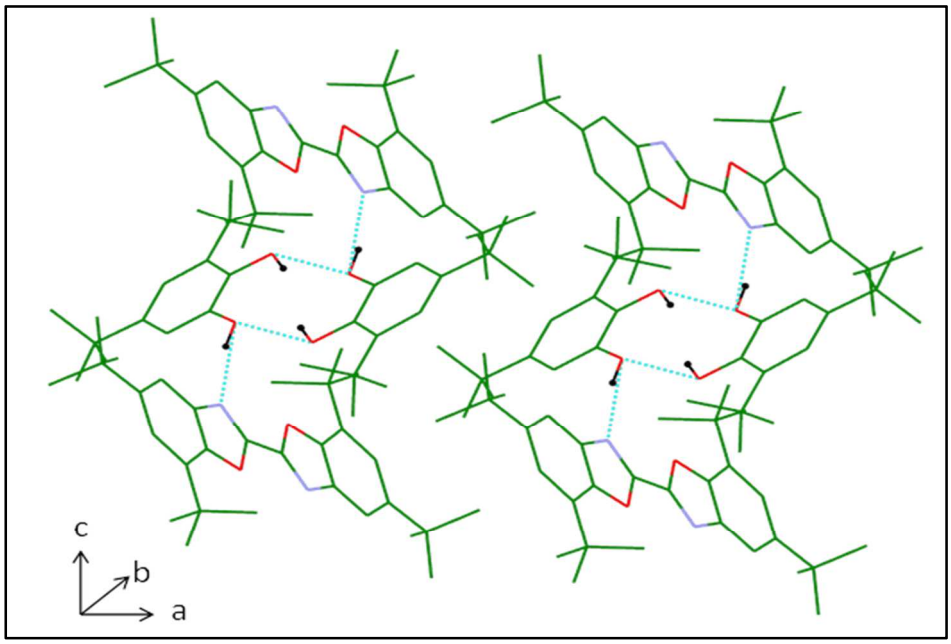


Figure S5. Powder XRD-data of cocrystals **2-4**

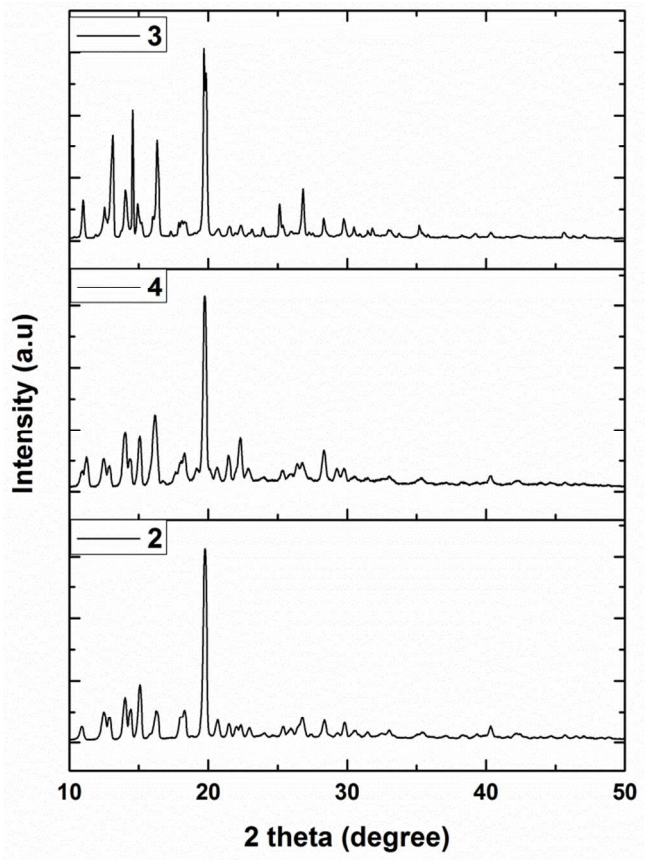


Figure S5A. Simulated powder XRD-data of cocrystals **2** from Mercury software 3.9 provided by CCDC

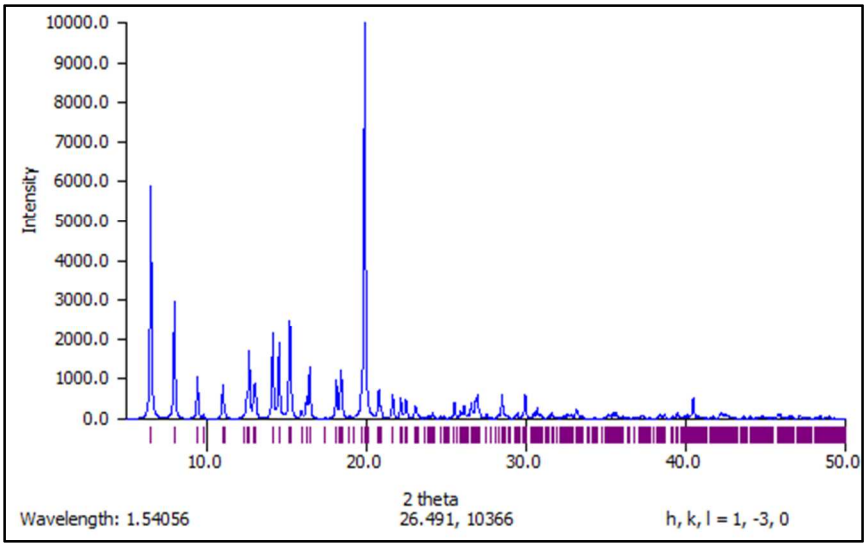


Figure S5b. DSC curve for **2**

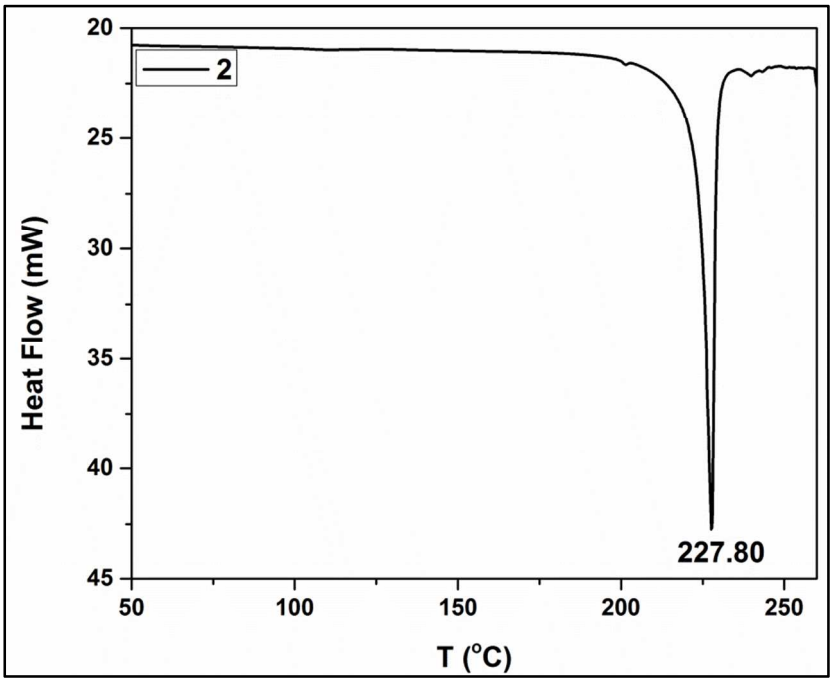


Figure S6. CO_2 absorption and desorption of **2**

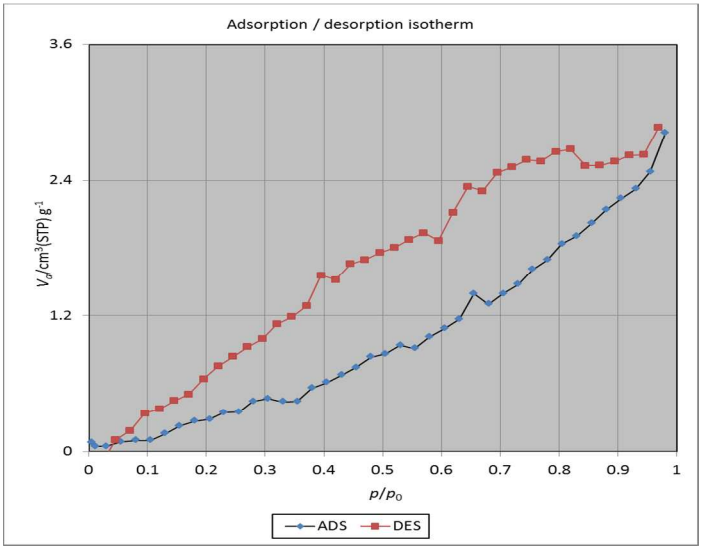


Figure S7. ^{1}H NMR spectrum of **3**

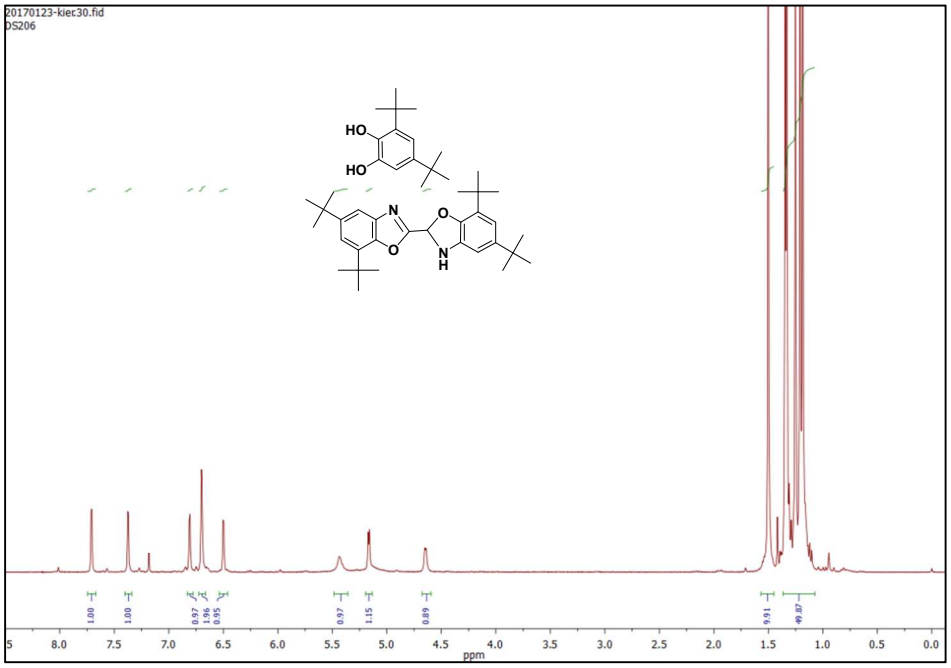


Figure S7A. ^{13}C NMR spectrum of **3**

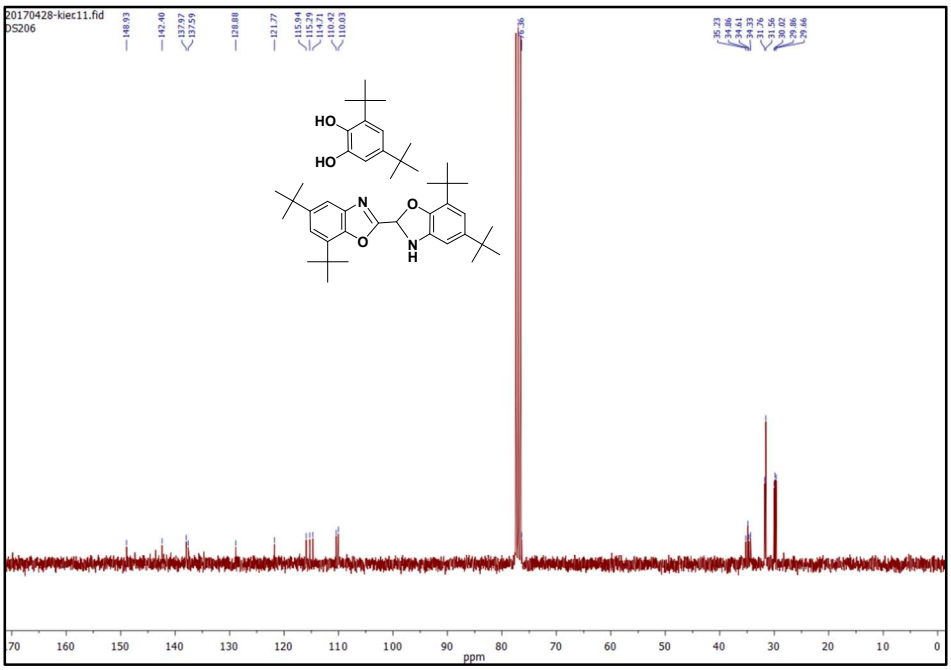


Figure S8. ^{1}H NMR spectrum of **4**

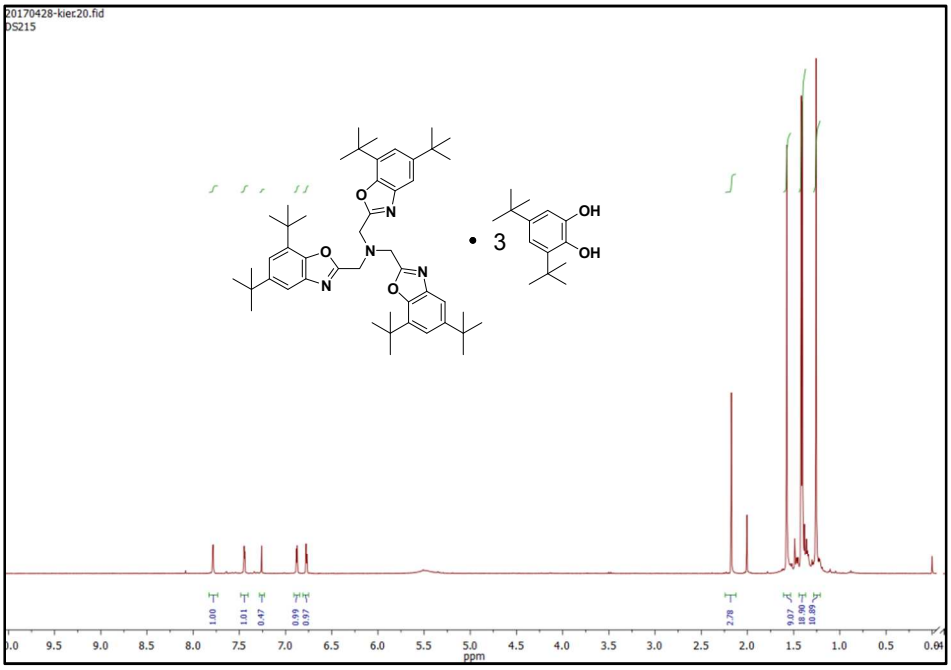


Figure S8A. ^{13}C NMR spectrum of **4**

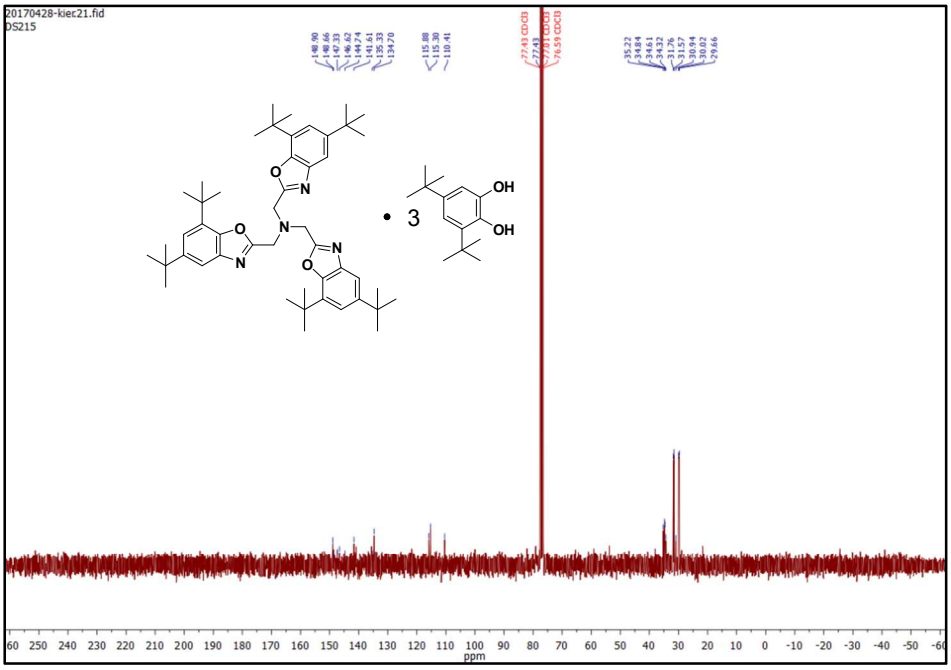


Figure S9. Mass data of **1**

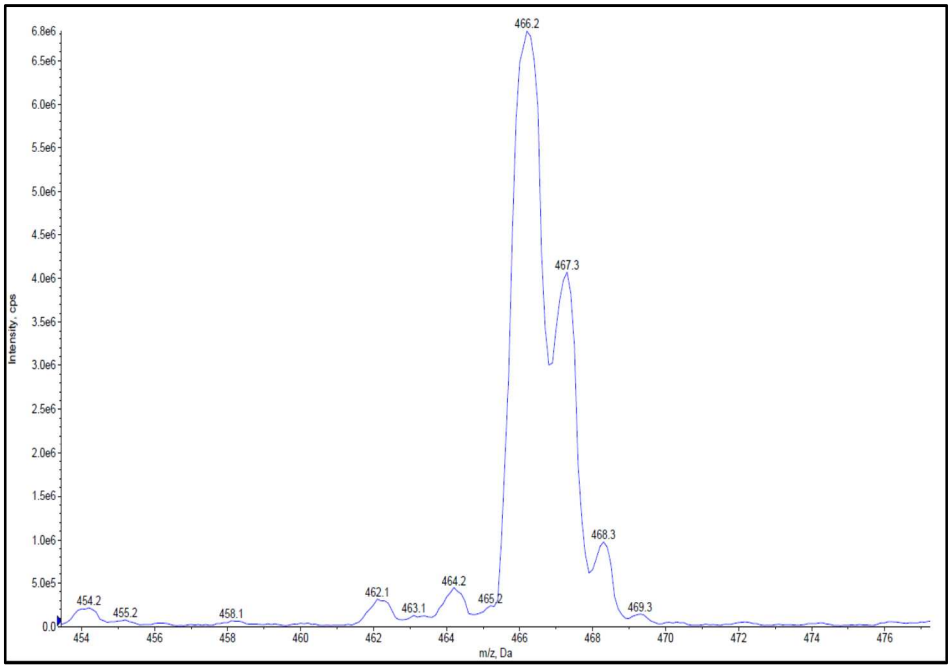


Figure S10. Mass data of **2**

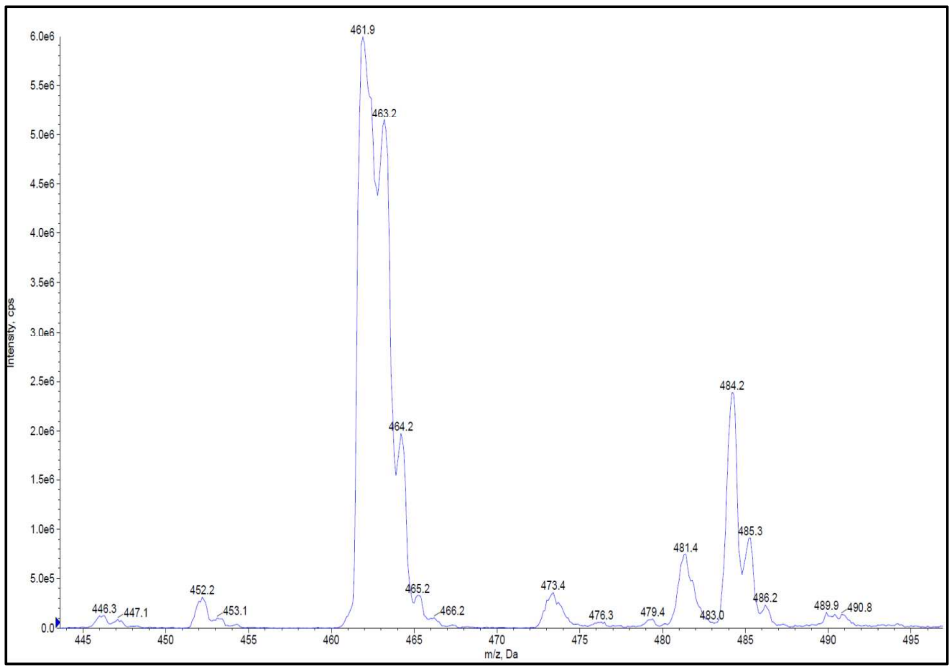


Figure S11. Mass data of **3**

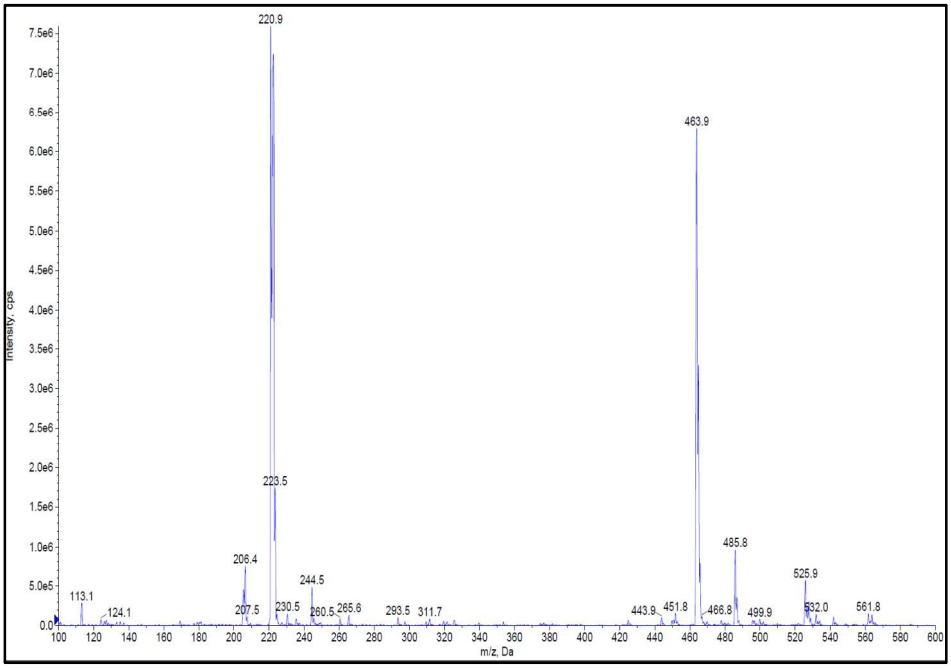


Figure S12. Mass data of **4**

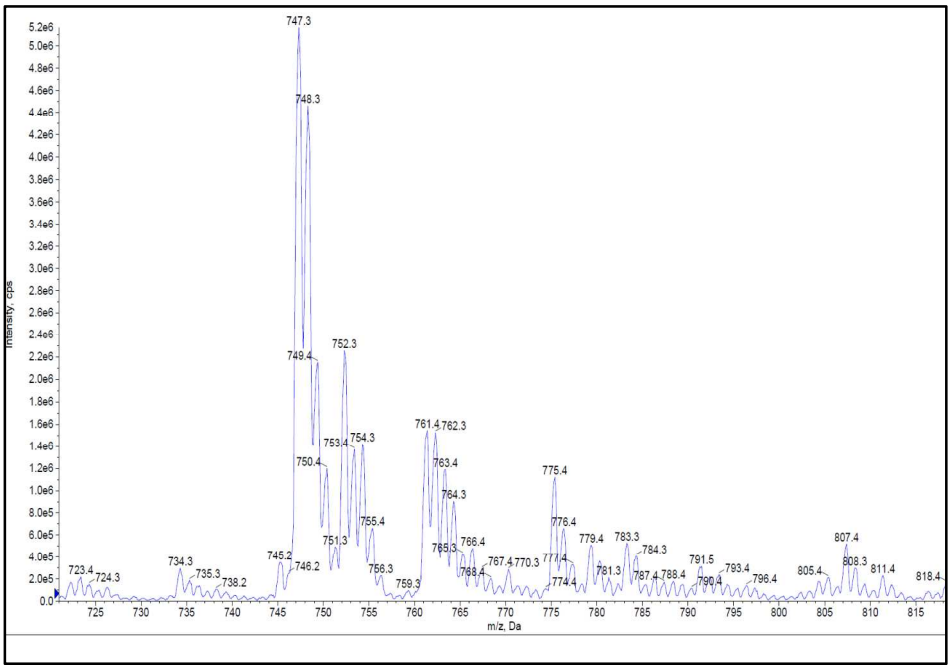


Table S1. Crystal data and structure refinement for **2**

CCDC	1533263	
Empirical formula	C29 H42 N O3	
Formula weight	452.64	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1035(2) Å	α= 79.8630(10)°
	b = 11.2303(2) Å	β= 81.5500(10)°
	c = 13.8595(2) Å	γ = 85.7350(10)°
Volume	1377.95(4) $Å^3$	
Z	2	
Density (calculated)	1.091 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	494	
Crystal size	0.30 x 0.29 x 0.27 mm^3	
Theta range for data collection	1.51 to 28.35°.	
Index ranges	-12<=h<=12, -14<=k<=14, -18<=l<=18	
Reflections collected	31105	
Independent reflections	6756 [R(int) = 0.0542]	
Completeness to theta = 28.35°	98.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6756 / 0 / 318	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1431	
R indices (all data)	R1 = 0.0662, wR2 = 0.1540	
Largest diff. peak and hole	0.235 and -0.238 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for **2**

Bond lengths [Å]		Bond angles [°]	
O(1)-C(1)	1.3588(13)	N(1)-C(1)-O(1)	116.16(10)
N(1)-C(1)	1.2903(15)	C(2)-C(3)-C(4)	121.22(11)
C(2)-O(1)	1.3834(14)	C(2)-C(3)-N(1)	108.63(10)
C(3)-N(1)	1.3935(16)	C(4)-C(3)-N(1)	130.15(10)
C(4)-C(3)	1.3891(17)	C(7)-C(6)-C(5)	125.60(11)
C(4)-C(5)	1.3828(17)	C(1)-O(1)-C(2)	103.52(8)

Table S3. Hydrogen bonds distance and angle in **2**

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A	Symmetry Code
O2-H2A	0.845	2.140	141.30	2.849	O3	[-x, -y, -z+1]
O3-H1A	0.821	1.979	164.87	2.780	N1	[-x+1, -y+1, -z+1]