Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Water Stabilizes Stacked Conformations of Ferrocene Containing Sheet-like Aromatic Oligoamides

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1) General Experimental Details

All solvents and starting reagents were purchased from commercial sources and used without further purification. When required, unless specifically mentioning, dry solvents were obtained directly prior to use by distillation from CaH_2 or sodium/benzophenone. Column chromatography was performed on silica gel (40-63 µm). Pyridine[1] monomers were synthesized according to published procedures. ^1H and ^{13}C nuclear magnetic resonance spectra were recorded on a Bruker Avance II 300 MHz spectrometer (^1H 300 MHz and ^{13}C 75 MHz) or a Bruker Avance 500 MHz spectrometer (^1H 500 MHz). Variable temperature NMR spectra were recorded on a Bruker Avance 600 MHz spectrometer (^1H 600 MHz). ^1H chemical shifts are reported in ppm relative to tetramethylsilane (TMS, δ = 0 ppm), Chloroform-*d* (δ = 7.26 ppm), Dichloromethane-d_2 (δ = 5.94 ppm). ^{13}C chemical shifts are reported in ppm using Chloroform-*d* (δ = 77.16 ppm), Dichloromethane -d_2 (δ = 5.94 ppm). High-resolution ESI mass spectra were recorded by the Mass Spectrometry service of the ASM platform of the Institute of Condensed Matter and Nanosciences at the Université catholique de Louvain.

X-ray crystallography

All diffraction data were recorded on a MAR345 image plate using Mo-Kα radiation generated by a Rigaku UltraX 18S rotating anode(Xenocs Fox3d mirrors). Prior to data collection the crystals were flash frozen to 150 K. Data integration and reduction was performed by CrysAlisPRO,[2] and the implemented absorption correction was applied. The structures were solved by SHELXT[3] and refined against F2 by SHELXL-2014/7.[4] All non-hydrogen atoms were re-fined anisotropically. Disorder was observed for all 3 THF solvent molecules and the THF molecules were modelled in two parts with refined occupancies of 50/50, 52/48 and 66/34.

The asymmetric unit contains two molecules of 1 and for one of them the terminal isobutyl groups were both disordered and refined in two discrete parts (66/34 and 72/28).

Hydrogen atoms were added in calculated positions and refined in riding mode, with temperature factors 1.2 times higher than their parent atoms (1.5 for methyl groups and water molecules). Hydrogen atoms of the lattice water molecules were located in the difference fourier maps after which the water molecules were idealized and refined as rigid groups allowed to translate with and/or rotated around the oxygen atom.

Isotropic and rigid bond restraints were applied to all disordered parts. Similarity restraints were applied between the major and minor disordered parts.

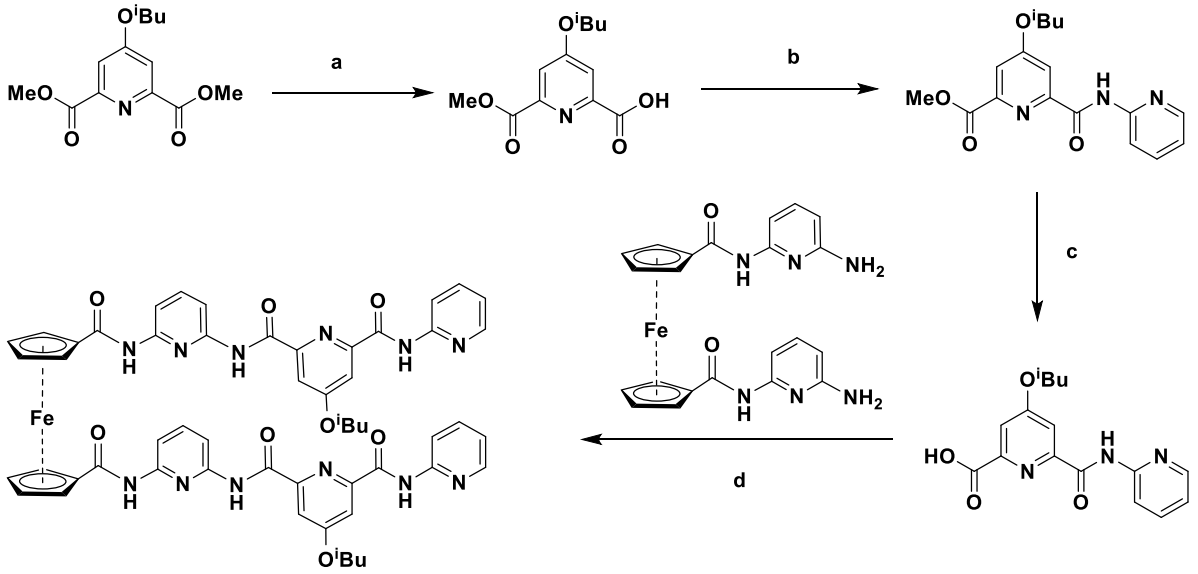
The crystal packing contains two large voids of 380Å in which no discrete molecules could be located, these voids were treated by the Squeeze algorithm in Platon to take in account the electron density of the heavily disordered regions.[5]

CSD 2071401 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from FIZ Karlsruhe via www.ccdc.cam.ac.uk/structures.

Computational Details

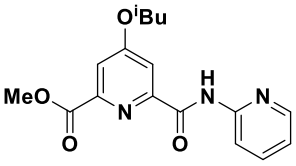
Computational modeling was performed with the Gaussian 09 software package[6] using the B3LYP-D3BJ[7] functional. All carbon, oxygen, nitrogen and hydrogen atoms were represented using the 6-311G*[8] basis set and the LANL2DZ[9] basis set was used for iron. Solvent effects (DCM) were included using the polarizable continuum model (PCM)

2) Synthetic schemes and experimental details



Scheme S1 Synthesis of oligomer **1**. a. NaOH; b. i. $(COCl)_2$, DMF, ii. 2-aminopyridine, Et_3N; c. NaOH; d. i. $(COCl)_2$, DMF, ii. $Fc(Pyr)_2$, Et_3N.

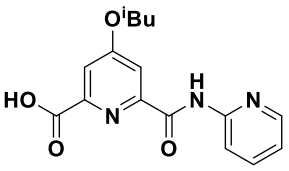
Dimethyl 4-isobutoxypyridine-2,6-dicarboxylate and its corresponding acid e were synthesized according to established procedures.[10]



Methyl 4-isobutoxy-6-(pyridin-2-ylcarbamoyl) picolinate : To a solution of 4-isobutoxy-6-(methoxycarbonyl) picolinic acid[9] (176 mg, 0.5 mmol) in 10 mL DCM, catalytic DMF followed by oxalyl chloride (0.43 mL, 5mmol) were added dropwise. The mixture was allowed to stir for 2 h. Solvent was removed by rotary evaporation. The solid was dried under vacuum for another 2 h and then used for the next step without further purification. The residue was suspended in 10 mL THF with 2-aminopyridine (47 mg, 0.5 mmol), and triethylamine (152 mg, 1.5 mmol) was added dropwise. The mixture was stirred at room temperature overnight. 30 mL of saturated sodium bicarbonate solution was added and extracted 3 times with 20 mL of DCM. The combined organic phases were dried over sodium sulfate and concentrated by rotary evaporation. The product was purified by column (PE/ EA = 5/1) to give the product as a white solid (130 mg, 78%).

^{1}H NMR (300 MHz, Chloroform-*d*) δ ^{1}H NMR (300 MHz, Chloroform-*d*) δ 10.41 (s, 1H), 8.46 – 8.21 (m, 2H), 7.88 (d, *J* = 2.5 Hz, 1H), 7.80 – 7.60 (m, 2H), 7.03 (ddd, *J* = 7.4, 4.9, 1.1 Hz, 1H), 3.96 (s, 3H), 3.86 (d, *J* = 6.5 Hz, 2H), 2.09 (dt, *J* = 13.3, 6.7 Hz, 1H), 0.99 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.83, 165.27, 162.16, 151.50, 151.15, 148.61, 148.35, 138.47, 120.22, 115.00, 114.35, 111.42, 75.40, 53.12, 28.16, 19.18.

HRMS (ESI): m/z calcd for $C_{17}H_{20}O_4N_3$, $[M+H]^+$ 330.13461, found 330.13466.



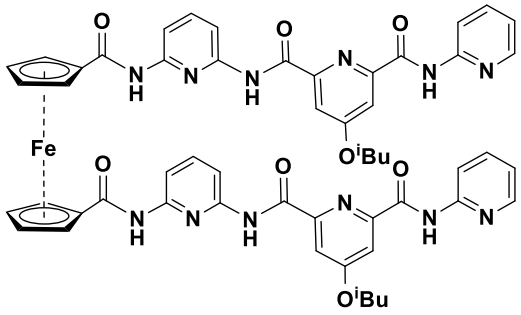
4-isobutoxy-6-(pyridin-2-ylcarbamoyl)picolinic acid: Methyl 4-isobutoxy-6-(pyridin-2-ylcarbamoyl)picolinate (100 mg, 0.3 mmol) was dissolved in 1,4-dioxane (6 mL) and methanol (2 mL) and cooled with an ice bath. Sodium hydroxide (12 mg, 0.3 mmol) dissolved in 1 mL of methanol was added to the mixture dropwise. After the addition was complete, the system was allowed to stir at room temperature for 4 h and monitored by TLC. 0.1 mL of acetic acid was added to the mixture followed by 10 mL of water and

the solution was extracted 3 times with 10 mL of DCM. The combined organic solution was dried over sodium sulfate and concentrated by rotary evaporation to afford the product as a white solid (79 mg, 80%).

^{1}H NMR (300 MHz, Chloroform-*d*) δ 11.29 (s, 1H), 8.56 (dt, *J* = 8.5, 0.9 Hz, 1H), 8.51 – 8.36 (m, 1H), 8.08 – 7.95 (m, 2H), 7.88 (ddd, *J* = 8.7, 7.4, 1.8 Hz, 1H), 7.19 (ddd, *J* = 7.4, 5.1, 1.0 Hz, 1H), 3.97 (d, *J* = 6.5 Hz, 2H), 2.19 (dt, *J* = 13.3, 6.7 Hz, 1H), 1.08 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 168.02, 167.40, 162.51, 150.90, 148.76, 146.59, 139.55, 120.18, 115.52, 114.19, 112.76, 75.42, 28.01, 19.05.

HRMS (ESI): m/z calcd for $C_{16}H_{18}O_4N_3$, $[M+H]^+$ 316.12957, found 316.12954.

Oligomer 1 : To a solution of 4-isobutoxy-6-(pyridin-2-ylcarbamoyl)picolinic acid (200 mg, 0.6 mmol) in freshly distilled DCM, a catalytic amount of anhydrous DMF was added followed by oxalyl chloride (813 mg, 6.4 mmol) and the reaction was stirred for 4 h at room temperature. Then the solvent was removed by rotary evaporation and the residue was dried under vacuum to give the acyl chloride, which was used without further purification. In a pre-dried round bottom flask under the protection of argon, the acyl chloride and ferrocene diamine[10] (137 mg, 0.3 mmol) were dissolved in chloroform. Triethylamine (71 mg, 0.7 mmol) was added dropwise at room temperature. The reaction was allowed to stir overnight. Then the solvent was removed by rotary evaporation and the mixture was purified by column (methanol/dichloromethane = 1/100) to afford **1** as an orange solid (183 mg, 58%). Single crystals of X-ray quality could be obtained by slow diffusion of hexane into a THF solution of **1** at 4 °C.



^{1}H NMR (300 MHz, Chloroform-*d*) δ 10.30 (s, 2H), 10.07 (s, 2H), 8.73 (s, 2H), 8.26 (d, J = 8.4 Hz, 2H), 8.12 – 7.98 (m, 2H), 7.86 (d, J = 8.1 Hz, 4H), 7.77 – 7.70 (m, 4H), 7.69 – 7.60 (m, 2H), 7.56 (t, J = 8.1 Hz, 2H), 6.98 – 6.89 (m, 2H), 5.12 (t, J = 1.9 Hz, 4H), 4.56 (t, J = 1.9 Hz, 4H), 3.94 (d, J = 6.6 Hz, 4H), 2.37 – 2.08 (m, 1H), 1.11 (d, J = 6.7 Hz, 12H). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 168.17, 167.19, 161.21, 160.74, 150.73, 150.14, 149.83, 148.57, 147.44, 140.64, 138.59, 78.48, 75.42, 72.27, 70.19, 28.07, 19.09.

HRMS (ESI): m/z calcd for $C_{54}H_{51}O_8N_{12}{}^{54}Fe$, $[M+H]^+$ 1049.33435, found 1049.33466.

3) Supporting Figures

Figure S1) Full ^{1}H-^{1}H ROESY spectrum of oligomer 1 in CD_2Cl_2

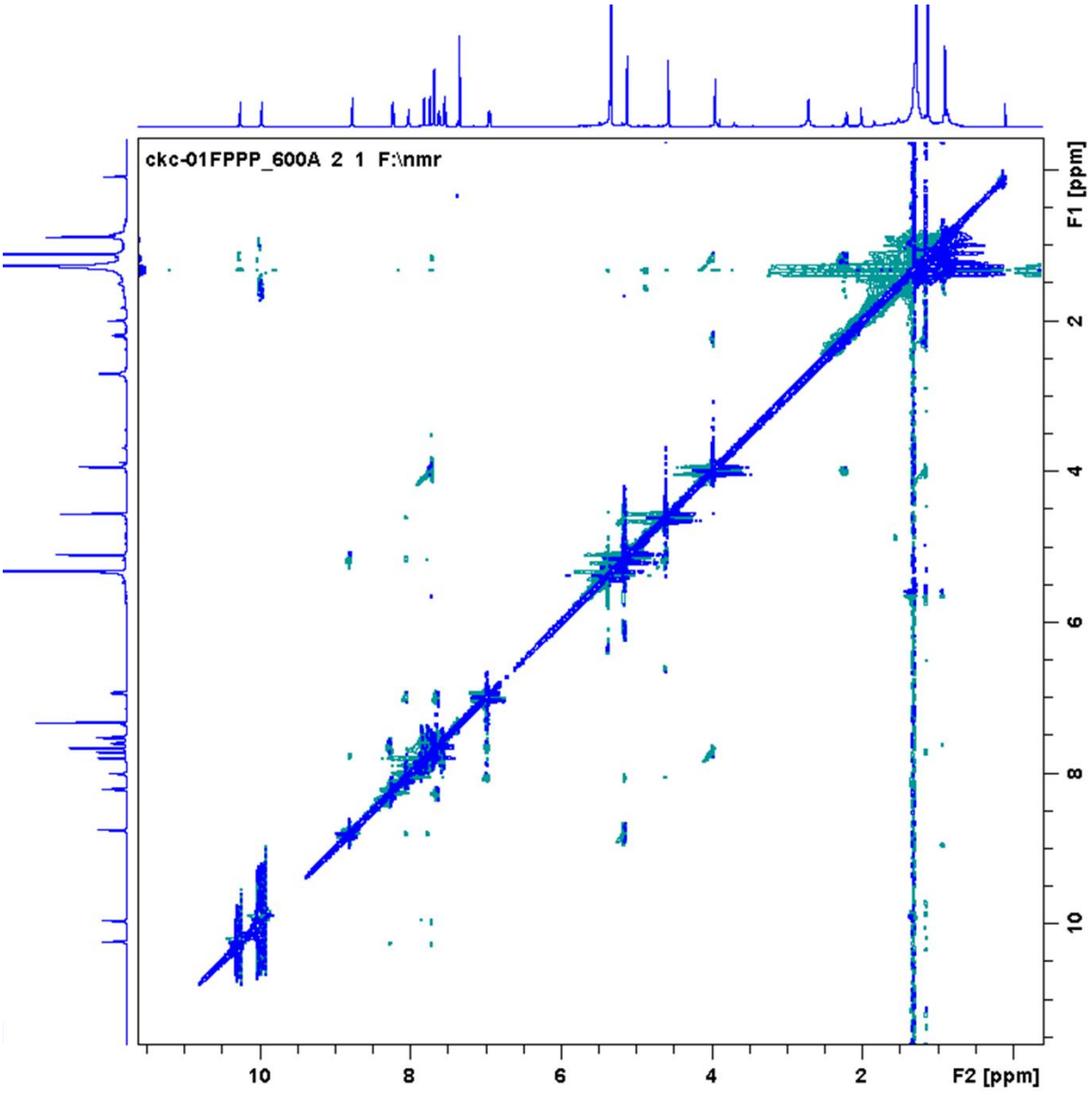


Figure S2) Full proton NMR spectrum for oligomer 1 (1mM in CD_2Cl_2) with variable concentrations of water. Water ratios were determined by integration.

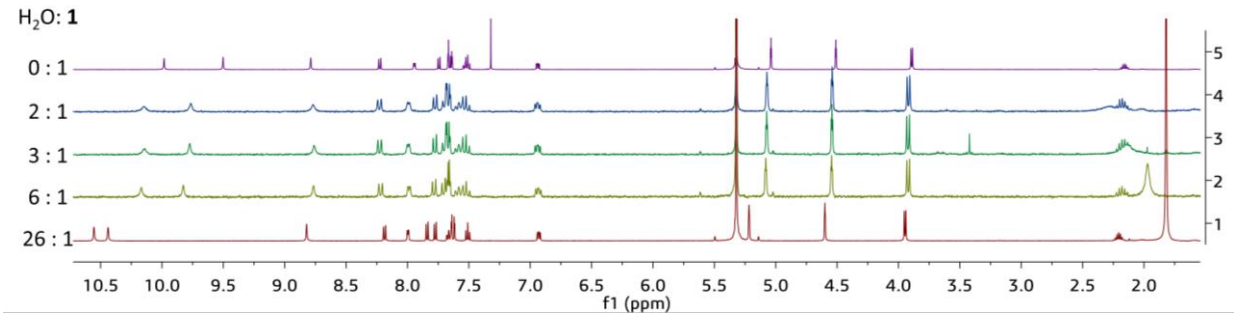


Figure S3) Full variable temperature ^1H NMR spectra of oligomer 1 (1mM) in CD_2Cl_2 containing water. (temperature range from 183 K to 298 K, from bottom to top)

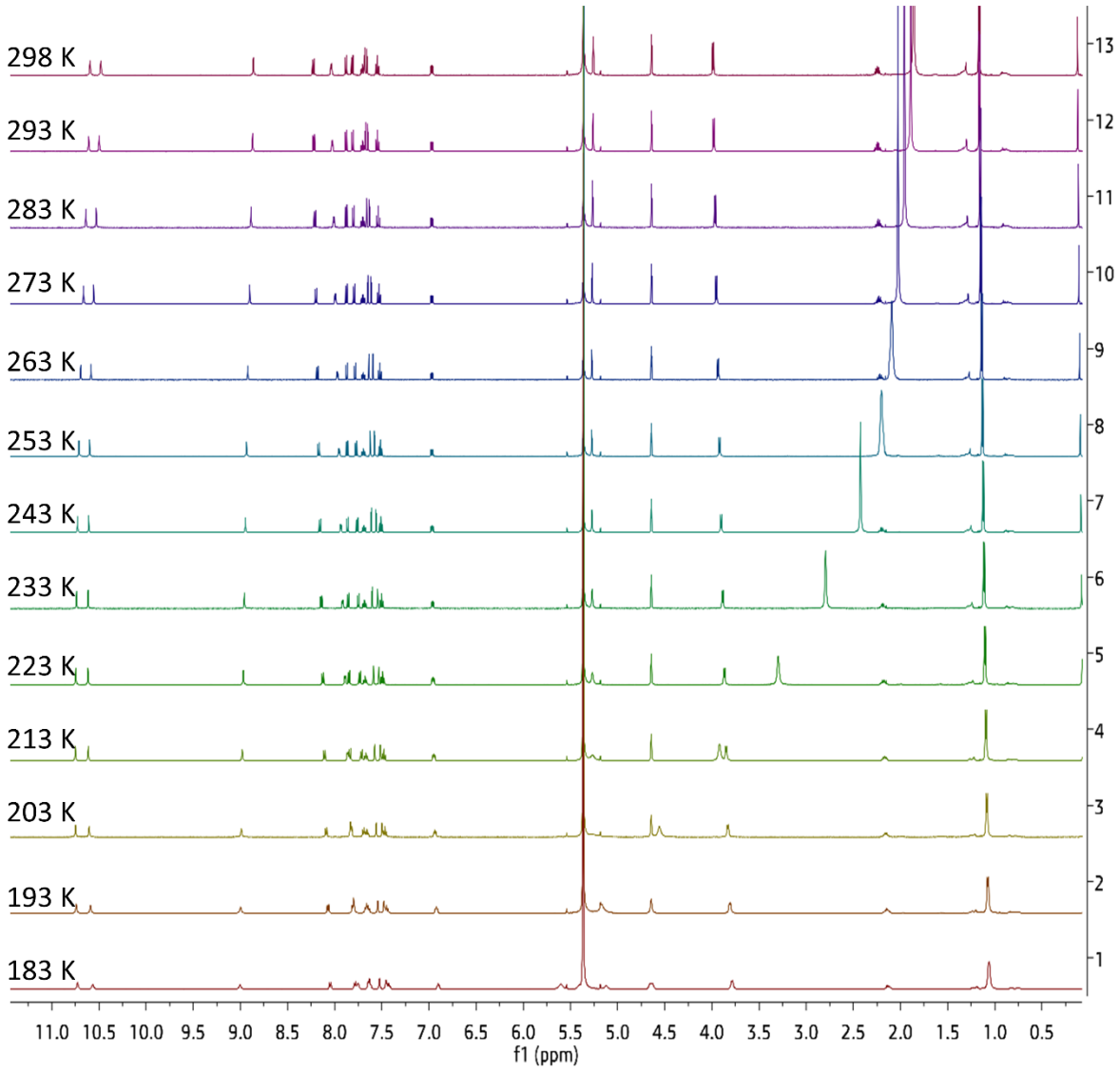
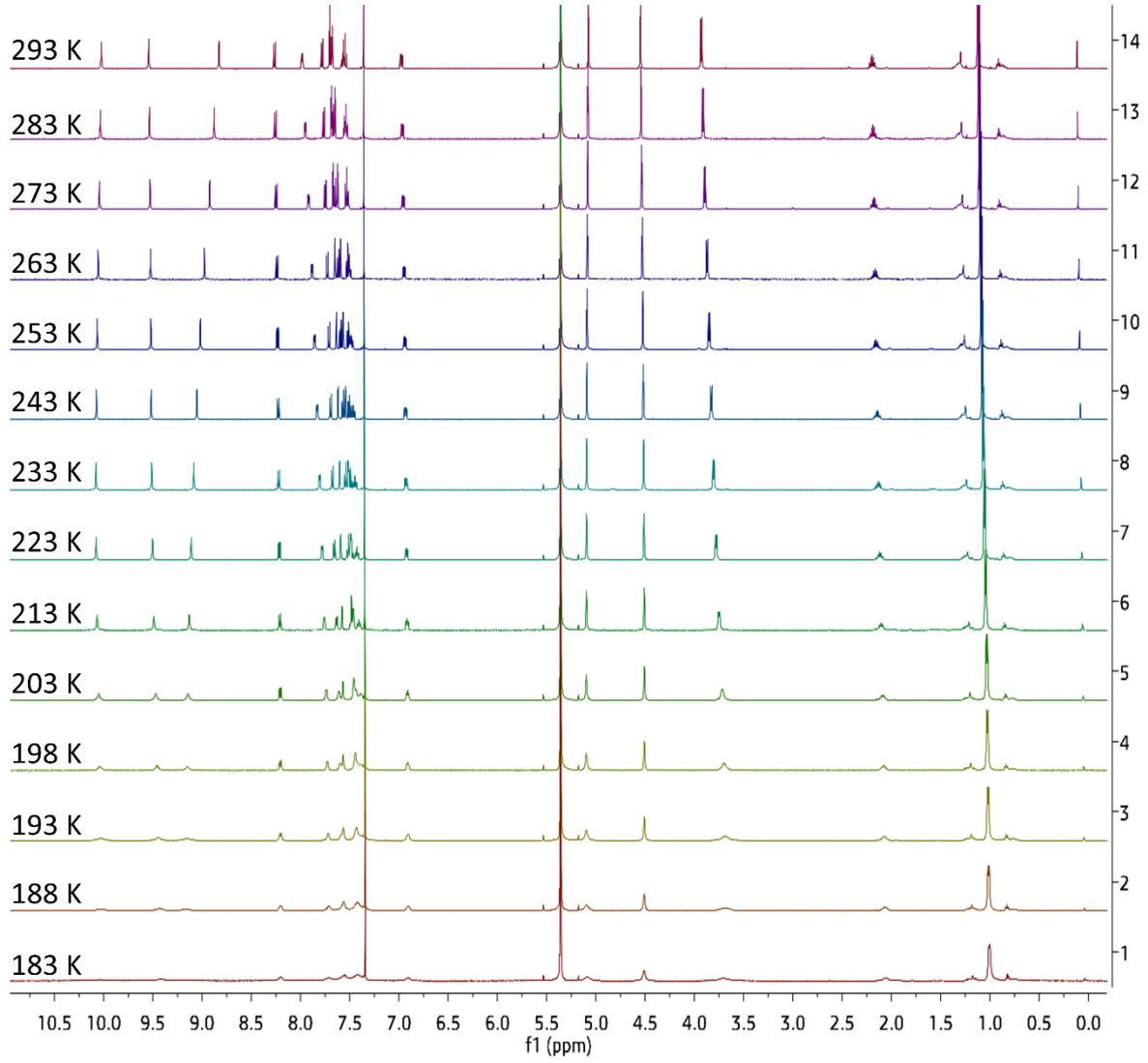


Figure S4) Full variable temperature ^{1}H NMR spectra of oligomer 1 (1mM) in anhydrous CD_2Cl_2 (temperature range from 183K to 293K, from bottom to top)



4) X-ray crystallographic data

Table S1 – X-ray crystallographic data for Oligomer 1

Parameter	**1**
CCSD #	2071401
Empirical formula	C120 H134 Fe2 N24 O24
Formula weight	2408.20
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P*21/*c*
Unit cell dimensions	a = 14.0152(3) Å b = 32.0600(7) Å c = 27.4484(5) Å β= 101.8778(18)°.
Volume	12069.2(4) Å3
Z	4
Density (calculated)	1.325 Mg/m3
Absorption coefficient	0.321 mm-1
F(000)	5064
Crystal size	0.50 x 0.35 x 0.10 mm3
Theta range for data collection	2.944 to 23.817°.
Reflections collected	48565
Independent reflections	18404 [R(int) = 0.0728]
Completeness to theta = 23.817°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.56765
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	18404 / 633 / 1788
Goodness-of-fit on F2	1.073
Final R indices [I>2sigma(I)]	R_1 = 0.0638, wR_2 = 0.1532
R indices (all data)	R_1 = 0.1062, wR_2 = 0.1741
Largest diff. peak and hole	0.567 and -0.462 e.Å-3

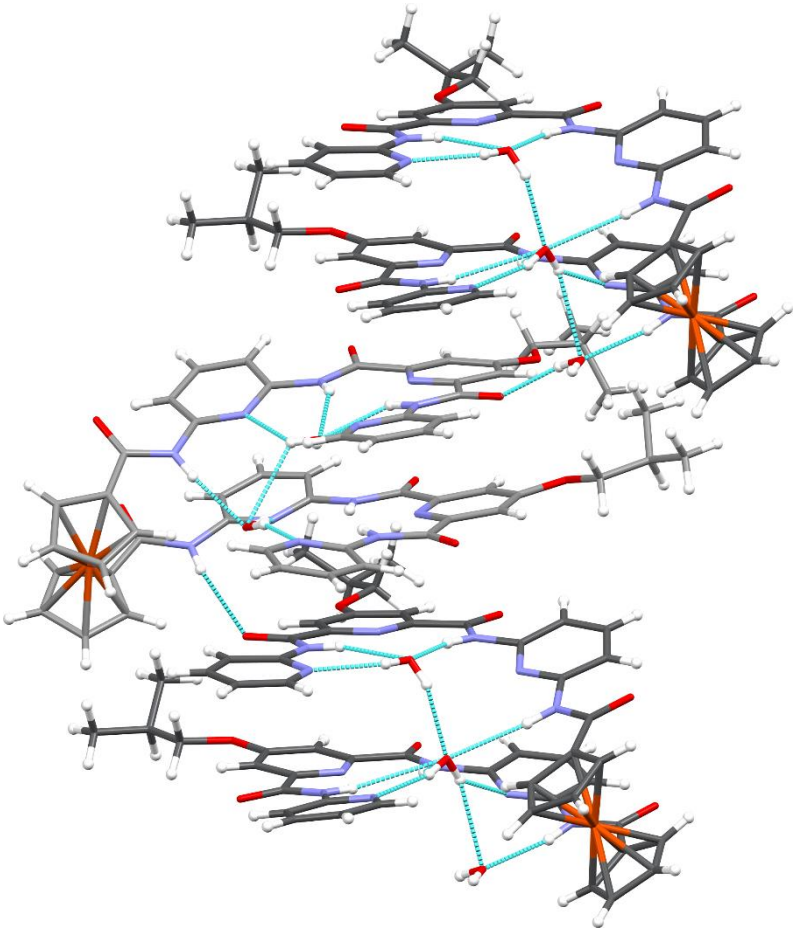


Figure S5 Crystal structure of oligomer **1** showing both intra- and intermolecular hydrogen bonding interactions

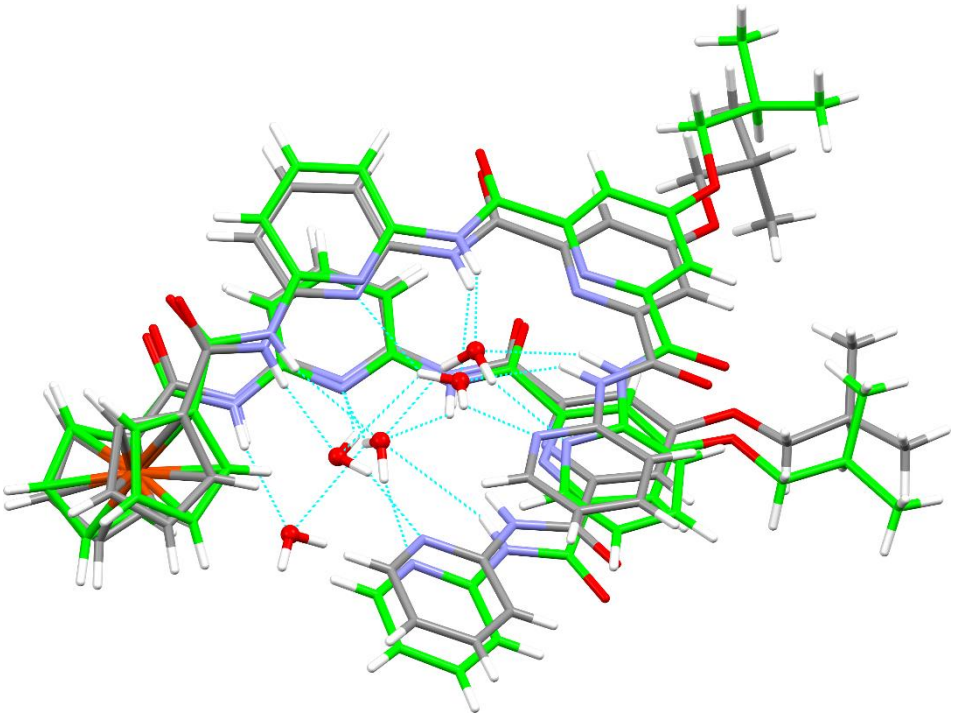


Figure S6 Overlay of the two independent molecules found in the unit cell.

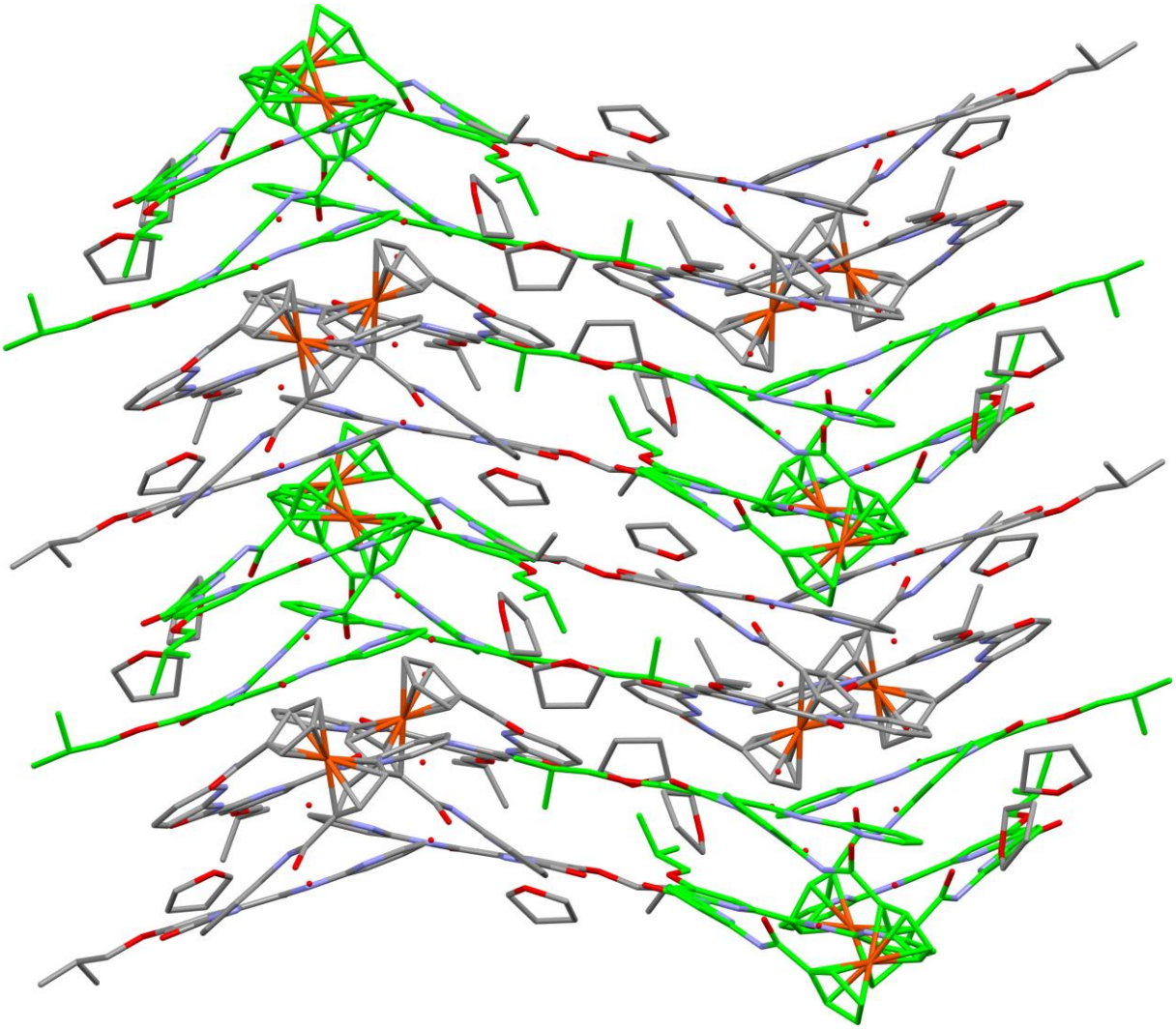


Figure S7 Packing of oligomer **1**

5) Computational study

Table S2 Coordinates of the optimized structures of **1**, **water dimer** and **water ⊂ 1** (Geometry optimization: B3LYP-D3BJ; 6-311G(d,p) for C,H,N,O and LANL2DZ for Fe

1

E = -8492468.67420 kJ/mol

Fe	-6.01571800	1.03830000	0.59069100
C	-7.51184500	-0.31903300	0.08194000
H	-7.77739000	-0.56190800	-0.93543600
C	-8.05210400	0.72732600	0.87760400
H	-8.80858000	1.43206200	0.56539400
C	-7.37189700	0.73396800	2.13210300
H	-7.53625500	1.43118800	2.94027200
C	-6.39866500	-0.30213000	2.11299100
H	-5.72118200	-0.55510600	2.91501400
C	-6.48285700	-0.95781600	0.83770600
C	-5.67775200	-2.12000300	0.38235800
O	-6.13062100	-3.00575800	-0.32588200
N	-4.38763100	-2.09657000	0.86098100
H	-4.07458500	-1.22996700	1.27612100
C	-3.35159200	-3.01847500	0.67958900
C	-3.51925200	-4.33458000	0.23640000
H	-4.49686500	-4.70616200	-0.02803000
C	-2.37381900	-5.12022800	0.14622100
H	-2.45867900	-6.14760900	-0.19084700
C	-1.11986100	-4.60677900	0.46561900
H	-0.21377100	-5.18743200	0.38391900
C	-1.07579800	-3.27317800	0.87736000
N	-2.16244400	-2.50735000	0.99772000
N	0.08878000	-2.56458400	1.17479200
H	-0.05944500	-1.56838400	1.28396000
C	1.38622400	-2.96438400	1.27293000
O	1.80081400	-4.10824000	1.15876300
C	2.29807400	-1.79399200	1.57606100
C	3.59695100	-2.01039700	2.00228600
H	3.99210400	-3.01371200	2.08698300
C	4.38796000	-0.89732200	2.32928000
C	3.82974400	0.37949800	2.20409000
H	4.37228000	1.28501100	2.43026800
C	2.53004500	0.48025400	1.71636100
N	1.77285600	-0.57071700	1.41556200
O	5.64552600	-1.14572000	2.72719400
C	6.48042600	-0.03144300	3.08730600
C	1.93858100	1.85203800	1.49403900
O	2.48325600	2.85304500	1.93682600
N	0.78773800	1.83400300	0.75507000
H	0.47925200	0.92594300	0.42202700
C	-0.00407500	2.91267600	0.34361600
N	-1.03698300	2.55452800	-0.43211600
C	-1.82959100	3.51892300	-0.91175800
H	-2.64996100	3.18718400	-1.53927000
C	-1.65309500	4.86795300	-0.63138000
H	-2.32651400	5.60770400	-1.04665200
C	-0.59406400	5.22383100	0.20141700
H	-0.41430200	6.26312700	0.45373000
C	0.25178300	4.24354800	0.70055300
H	1.09615200	4.48490200	1.32528500
C	-5.49942400	2.09801400	-1.09937100
H	-6.01157900	2.00955300	-2.04498200
C	-5.79828700	3.00362400	-0.04535500
H	-6.59945200	3.72777900	-0.04266200
C	-4.90496800	2.74096500	1.03565900
H	-4.91505100	3.22899100	1.99896300
C	-4.04154900	1.67887800	0.65077000
H	-3.25760600	1.24590400	1.25326800
C	-4.40218900	1.28103600	-0.67804500
C	-3.83378500	0.18627800	-1.50319200
O	-4.53151600	-0.45450800	-2.27958000
N	-2.48753400	-0.02393400	-1.31353400
H	-1.94482800	0.71108100	-0.85277700
C	-1.71978500	-1.08145300	-1.81674100
C	-2.27248800	-2.21320500	-2.43302100
H	-3.33619700	-2.29308500	-2.57985000
C	-1.40088700	-3.21979100	-2.81933700
H	-1.79497500	-4.11903200	-3.27967600
C	-0.03137400	-3.09664200	-2.61481100
H	0.66683800	-3.86706800	-2.89810700
C	0.41098100	-1.92437900	-1.99912500
N	-0.40676100	-0.94143700	-1.60348800
N	1.75789700	-1.66279000	-1.72074900

H_2O

E = -401372.62894 kJ/mol

O	-1.46237500	0.08749300	0.07537200
H	-0.49420100	0.14452400	-0.02108100
H	-1.72963100	-0.64514900	-0.48872900
O	1.32128400	-0.05222200	-0.09486100
H	1.55354900	-0.56267200	0.68809300
H	1.79901600	0.78113400	-0.02236800

$H_2O \subset 1$

E = -8893908.11161 kJ/mol

Fe	6.22498400	0.74902400	-0.39570400
C	7.20868600	-0.99561700	-0.93443600
H	7.61115700	-1.70937500	-0.23281600
C	7.87595900	0.12423200	-1.49521500
H	8.88883700	0.43052300	-1.27944600
C	6.95533200	0.81739700	-2.33754000
H	7.15228400	1.73208400	-2.87687800
C	5.71196700	0.13011700	-2.29833700
H	4.81649400	0.42325000	-2.82603400
C	5.86354300	-1.00124800	-1.42669300
C	4.88323300	-2.06154100	-1.09233900
O	5.23382800	-3.11937700	-0.58868800
N	3.57626300	-1.76550700	-1.42337300
H	3.36007400	-0.79823100	-1.63032100
C	2.45582800	-2.60123200	-1.36211400
C	2.51588900	-3.98110900	-1.13418900
H	3.46051800	-4.46325300	-0.94610400
C	1.31638100	-4.68096300	-1.13661300
H	1.32420100	-5.74958800	-0.95260000
C	0.10526600	-4.03563000	-1.36034700
H	-0.83830000	-4.55642500	-1.35181400
C	0.15511400	-2.65597700	-1.56368000
N	1.29802700	-1.95811700	-1.56496000
N	-0.97235700	-1.85507200	-1.74965200
H	-0.80917200	-0.85439800	-1.74866300
C	-2.28337600	-2.21230700	-1.87213400
O	-2.71676000	-3.35505500	-1.89348300
C	-3.19258400	-1.00962500	-1.95193100
C	-4.55740400	-1.18916400	-2.09725900
H	-4.97852000	-2.18235300	-2.17245800
C	-5.38297600	-0.05621300	-2.08743700
C	-4.78859900	1.20222600	-1.96743900
H	-5.35282200	2.12204200	-1.94292100
C	-3.40236300	1.26316400	-1.83376700
N	-2.61516400	0.19242100	-1.82508300
O	-6.70880800	-0.27471700	-2.15339800
C	-7.59240400	0.84995200	-2.01622200
C	-2.75372500	2.61670300	-1.66873500
O	-3.37376900	3.64248600	-1.91491000
N	-1.46293800	2.55438100	-1.22466600
H	-1.12602700	1.64225300	-0.91624900
C	-0.58248600	3.61288800	-0.98419500
N	0.64011600	3.21828000	-0.59606500
C	1.54880000	4.15353700	-0.29964100
H	2.51841800	3.78594700	0.02131700
C	1.29936500	5.51691000	-0.38491200
H	2.06977600	6.23439100	-0.13048800
C	0.03402600	5.91771300	-0.81042200
H	-0.21109900	6.97077600	-0.89448200
C	-0.92808000	4.96549200	-1.11506100
H	-1.92248900	5.24041400	-1.42621100
C	6.51303700	1.11329500	1.62452500
H	7.16092900	0.52984700	2.25925300
C	6.85949400	2.26984600	0.87870100
H	7.83812200	2.72439700	0.83399000
C	5.70889500	2.68521500	0.14346800
H	5.66596900	3.50789400	-0.55540400
C	4.64736200	1.78409000	0.42762800
H	3.67545800	1.78307200	-0.03492200
C	5.14173000	0.80282300	1.35365600
C	4.48333200	-0.39101500	1.94101600
O	5.08988400	-1.10753600	2.72971200
N	3.18460400	-0.61650600	1.54715700
H	2.74825000	0.01591600	0.87004600
C	2.38944400	-1.71895300	1.88958400
C	2.89836500	-2.91762800	2.40330600
H	3.95249600	-3.02547100	2.59397200
C	1.99975100	-3.95150900	2.62652700
H	2.36189800	-4.89903400	3.01069800
C	0.64711800	-3.79816400	2.34981400
H	-0.06395700	-4.59390600	2.49895200
C	0.23413400	-2.55952300	1.85132800
N	1.08514400	-1.54633100	1.63198200
N	-1.10177800	-2.24685000	1.56534600

H	1.94268400	-0.74408400	-1.33811400
C	2.84098000	-2.48418000	-1.84649700
O	2.82370900	-3.63325900	-2.26154900
C	4.12031900	-1.83678300	-1.37307900
C	5.22387300	-2.63601800	-1.12441300
H	5.17768900	-3.70425000	-1.28657200
C	6.38857400	-2.03716600	-0.62688400
C	6.39007000	-0.65202200	-0.42798300
H	7.24597400	-0.11163700	-0.05216700
C	5.22636200	0.05338700	-0.71892300
N	4.10960400	-0.51216000	-1.17790800
O	7.41940500	-2.85488500	-0.36747800
C	5.19868800	1.54422400	-0.47242000
O	6.08817500	2.10258300	0.15962300
N	4.10375600	2.14792500	-1.00795500
H	3.47167400	1.54065200	-1.51664400
C	3.73511900	3.49988300	-1.01741200
N	2.64588800	3.73034100	-1.75891600
C	2.20151700	4.98641000	-1.83977200
H	1.30799600	5.13309200	-2.43904000
C	2.81218300	6.05936400	-1.19846600
H	2.40927400	7.06032300	-1.29665300
C	3.94278300	5.79952700	-0.42591200
H	4.44822700	6.60262000	0.09955000
C	4.42385000	4.50042700	-0.32181400
H	5.29117600	4.25471600	0.27059200
C	8.60459000	-2.30390800	0.22341000
H	7.44179500	-0.46428100	3.35095200
H	6.06669700	0.49597200	3.94989600
H	6.59562900	0.65656300	2.24703200
H	9.27670800	-3.14591000	0.36505100
H	8.37646700	-1.84760000	1.18958400
H	9.06907600	-1.57013300	-0.43967800
Fe	-6.01571800	1.03830000	0.59069100
C	-7.51184500	-0.31903300	0.08194000
H	-7.77739000	-0.56190800	-0.93543600
C	-8.05210400	0.72732600	0.87760400
H	-1.29454100	-1.26204400	1.38565500
C	-2.17244700	-3.09464200	1.50540100
O	-2.12568500	-4.31168200	1.61324100
C	-3.48800400	-2.38013100	1.29392000
C	-4.62831400	-3.11884100	1.02262000
H	-4.57839400	-4.19490900	0.92883500
C	-5.84179900	-2.44031200	0.84623500
C	-5.85439500	-1.04769600	0.98651800
H	-6.74805500	-0.45189800	0.87775600
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N	-3.48728800	-1.04635200	1.39003200
O	-6.91026500	-3.19141900	0.53545400
C	-4.61786700	1.10089900	1.34849300
O	-5.63851200	1.77195500	1.26694000
N	-3.35345200	1.58187600	1.52618300
H	-2.62369200	0.87223500	1.53010900
C	-2.92168200	2.88874100	1.76820700
N	-1.60534000	2.97540100	2.01816700
C	-1.08631200	4.17793700	2.28066100
H	-0.01620100	4.20081600	2.45973600
C	-1.84101800	5.34389700	2.30944100
H	-1.37189300	6.29615700	2.52346200
C	-3.20292300	5.24538900	2.03085300
H	-3.82903800	6.13086500	2.02439300
C	-3.76508800	4.00657100	1.74988300
H	-4.81316800	3.89030700	1.52281500
O	-0.59588400	0.60172800	0.80119700
H	0.20327200	0.08188800	1.01573900
H	-0.60349100	1.40995200	1.34972500
O	1.95149900	0.68571800	-0.72118800
H	1.36674300	1.47313900	-0.68898700
H	1.44175400	-0.07803400	-1.04831000
C	-8.14856800	-2.53036000	0.23273200
H	-8.59656200	0.43502500	-2.03929100
H	-7.46536800	1.54881500	-2.84578500
H	-7.41990800	1.35926800	-1.06493000
H	-8.84012300	-3.32266500	-0.04125300
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H	-8.53084100	-1.99595500	1.10603700

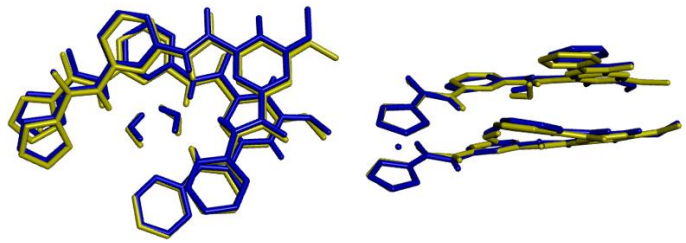


Figure S8 Top and side view of comparison of crystal structure (blue) with calculated structure (yellow)

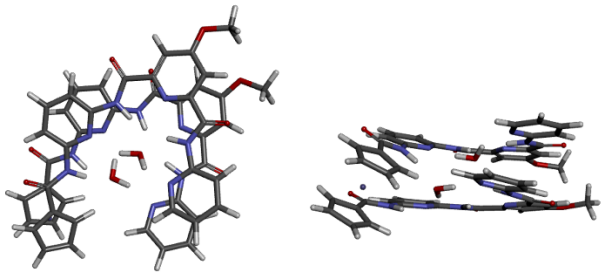


Figure S9 Top and side view of calculated structure of oligomer **1** with water molecules

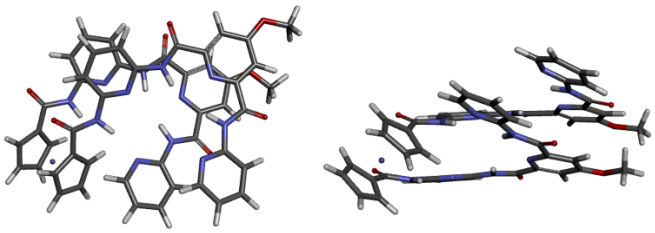
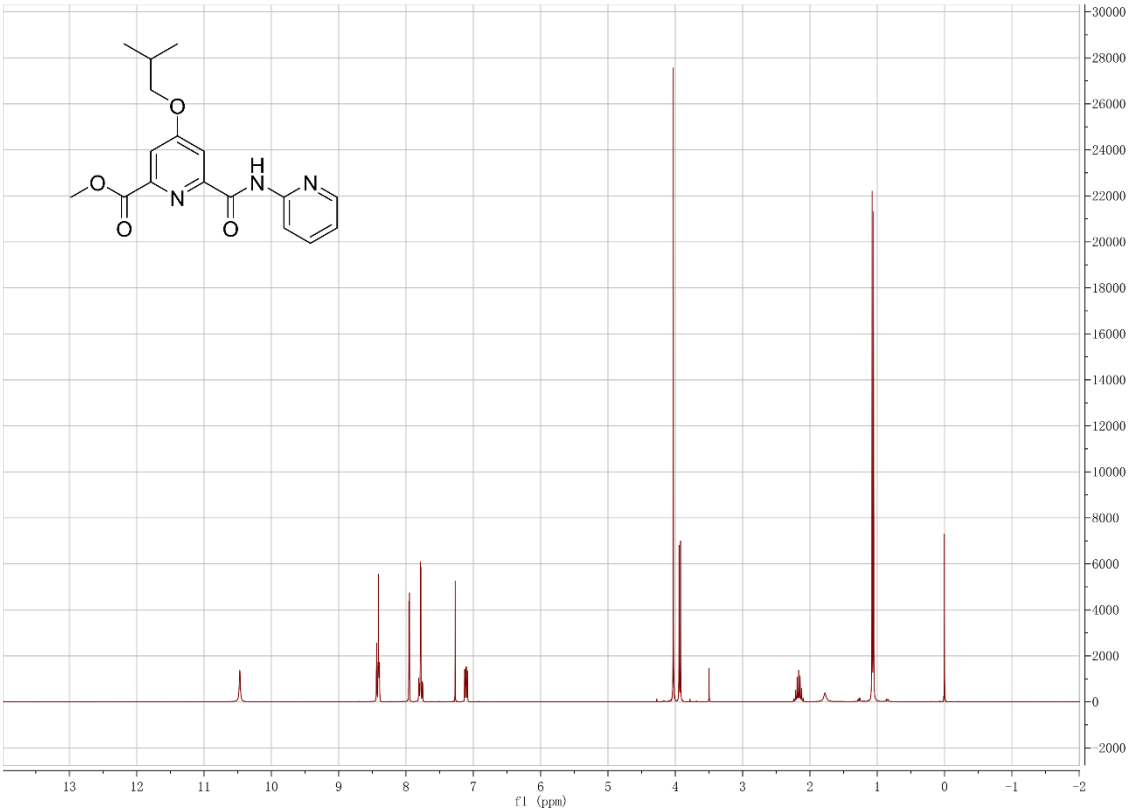


Figure S10 Top and side view of calculated structure of oligomer **1**

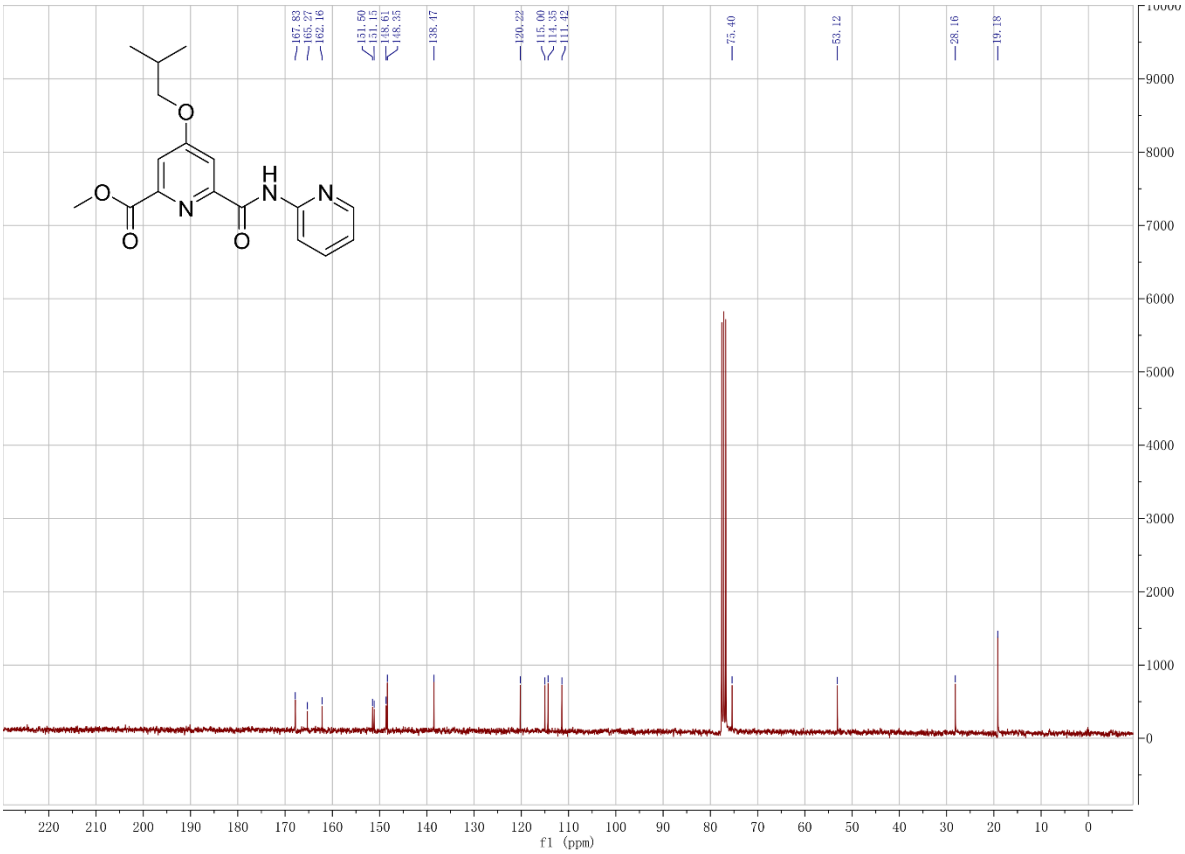
Figure S11 Top and side view of calculated structure of water molecules

6) NMR Spectra

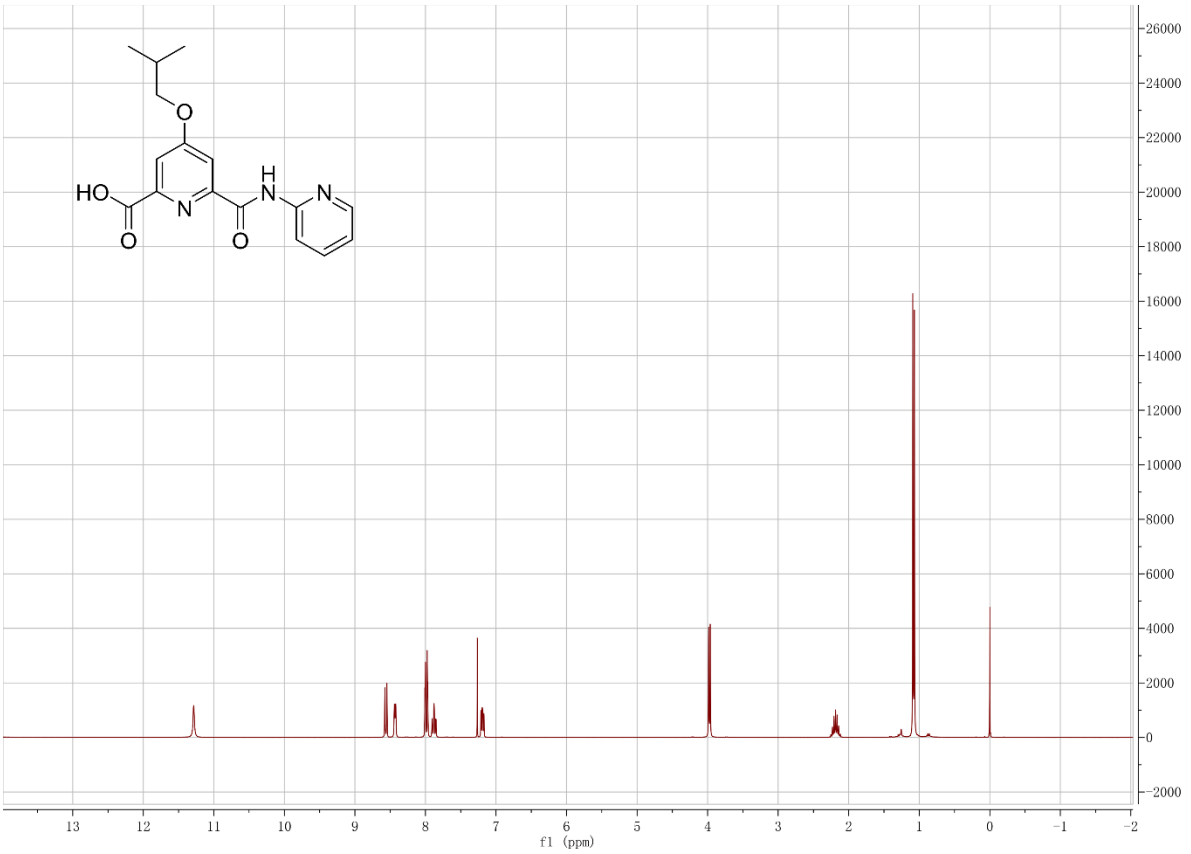
S12 Proton NMR of **Dimer ester**



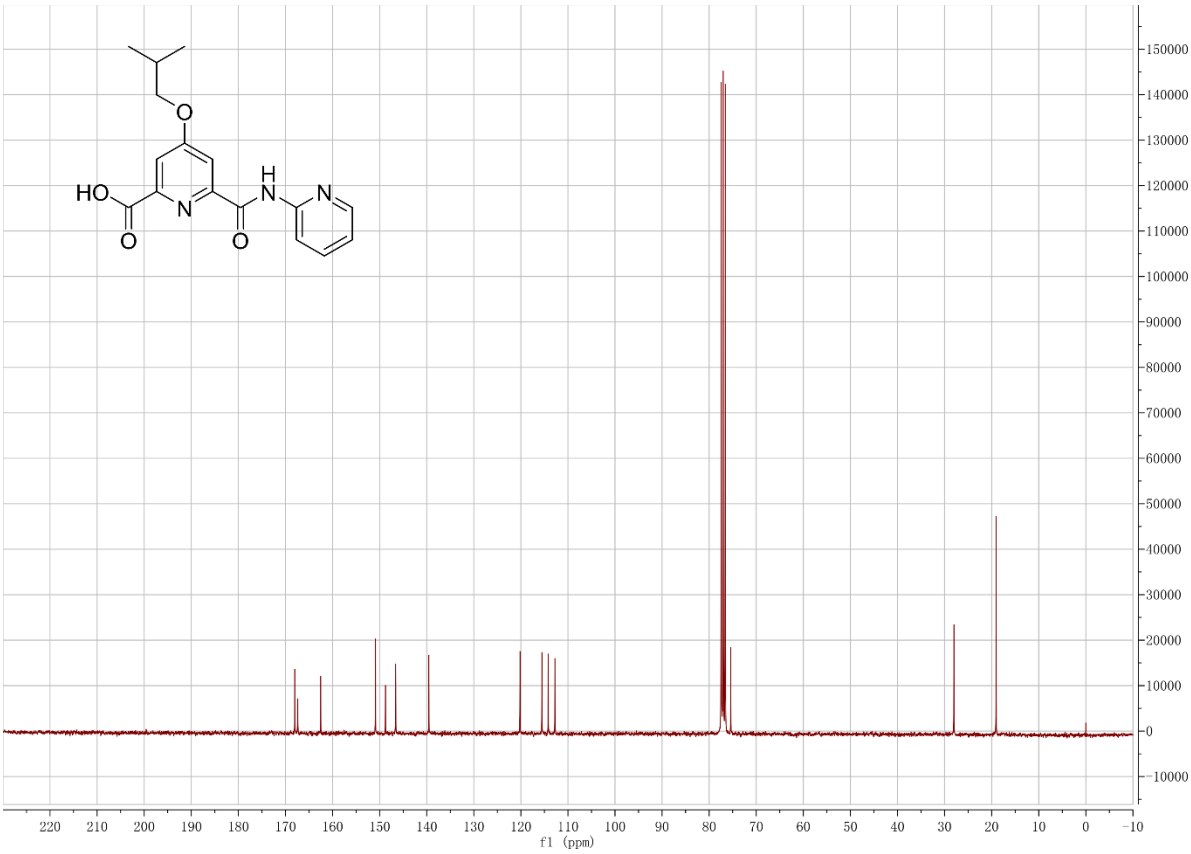
S13 Carbon NMR of **Dimer ester**



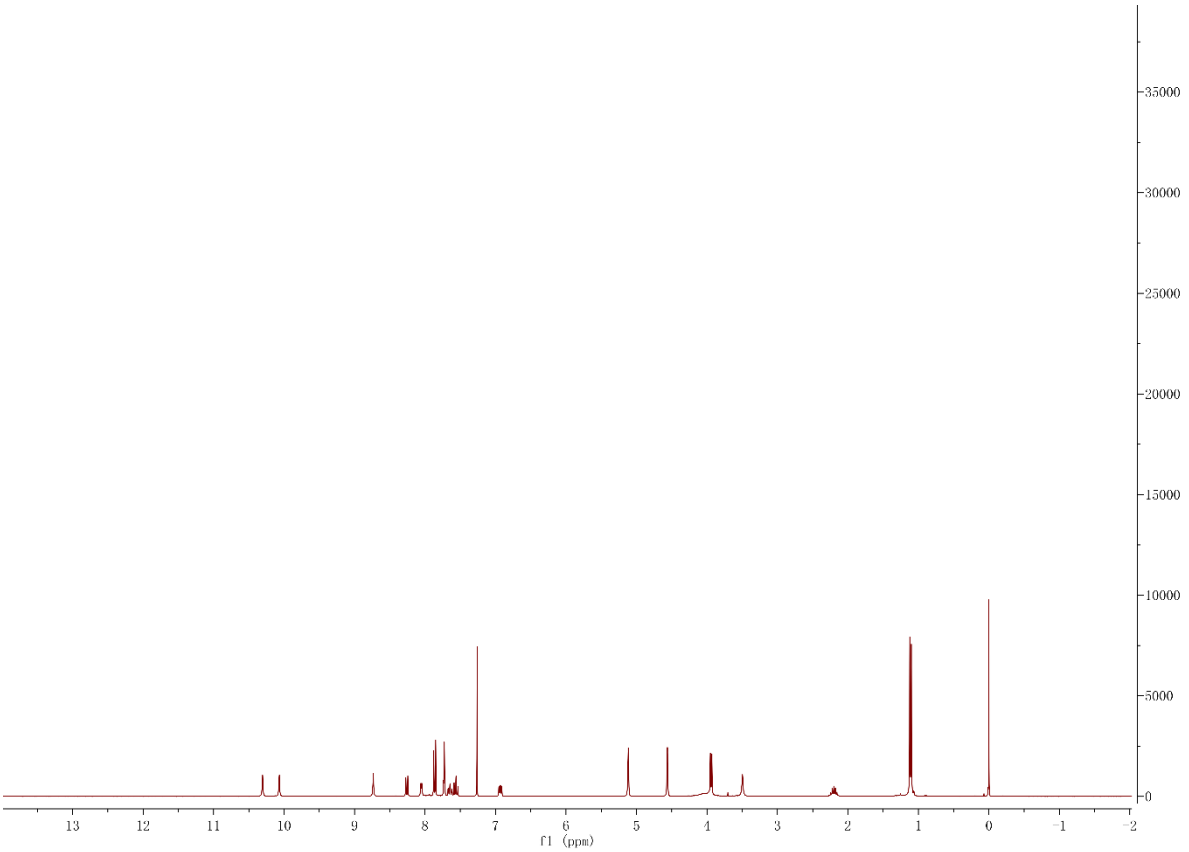
S14 Proton NMR of **Dimer acid**



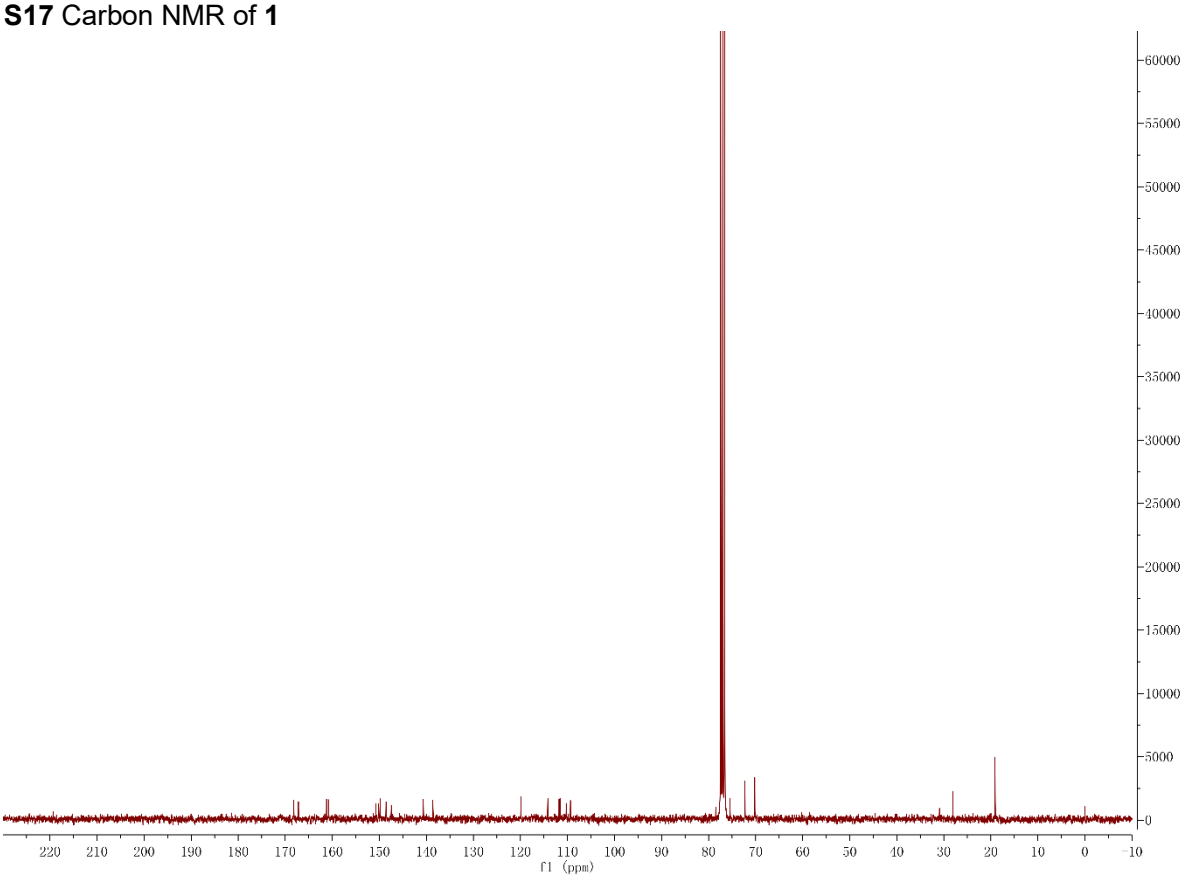
S15 Carbon NMR of **Dimer acid**



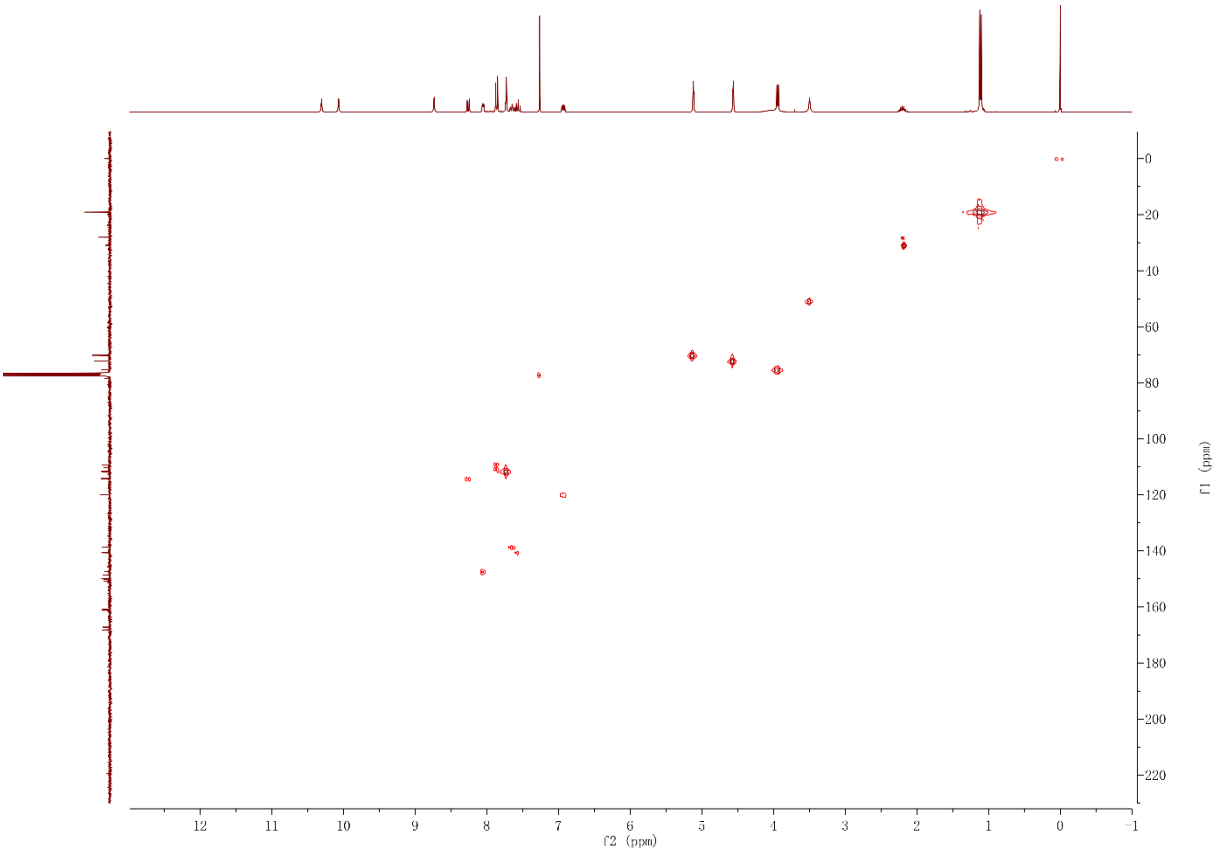
S16 Proton NMR of **1**



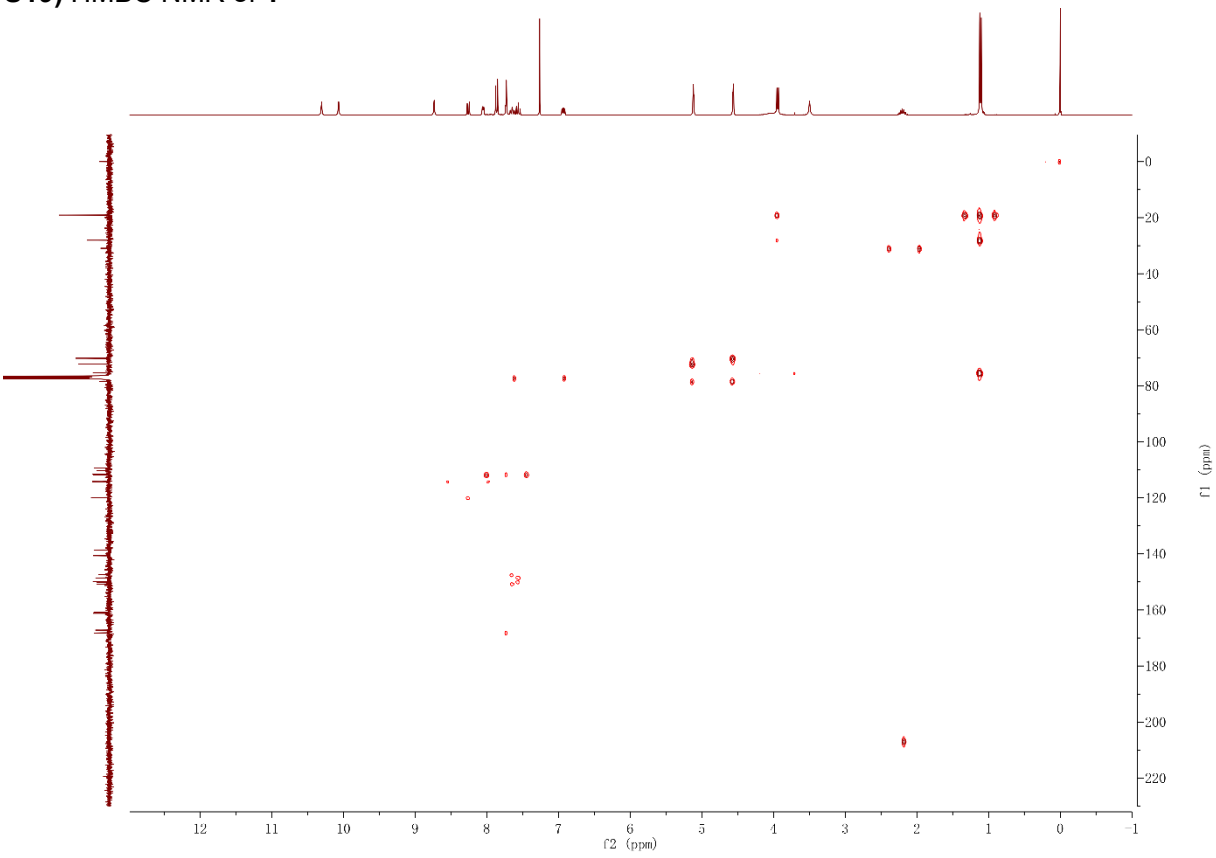
S17 Carbon NMR of **1**



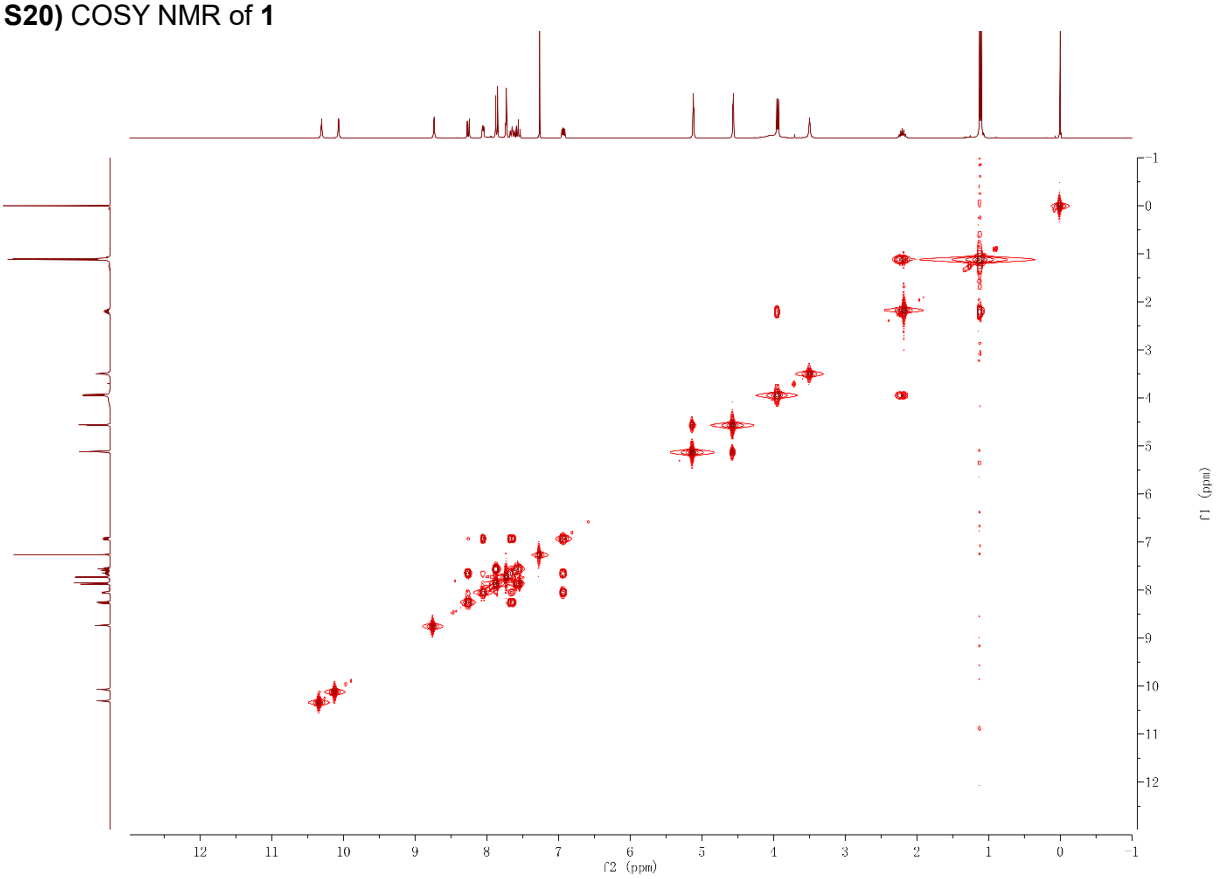
S18 HMQC NMR of **1**



S19) HMBC NMR of **1**



S20) COSY NMR of **1**



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