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Supporting Information

Phosphorescent Thymidine Triphosphate Sensor based on Donor and Acceptor Ensemble System via Intermolecular Energy Transfer

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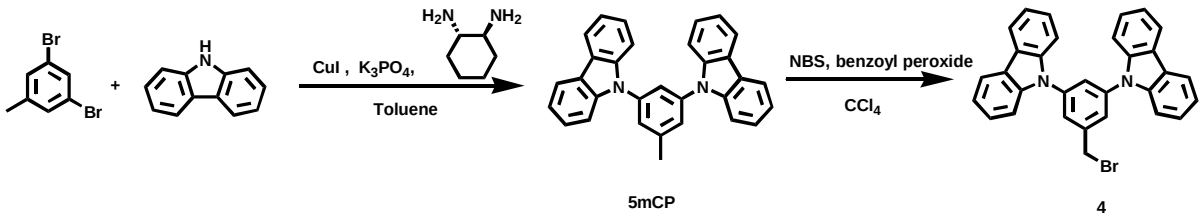
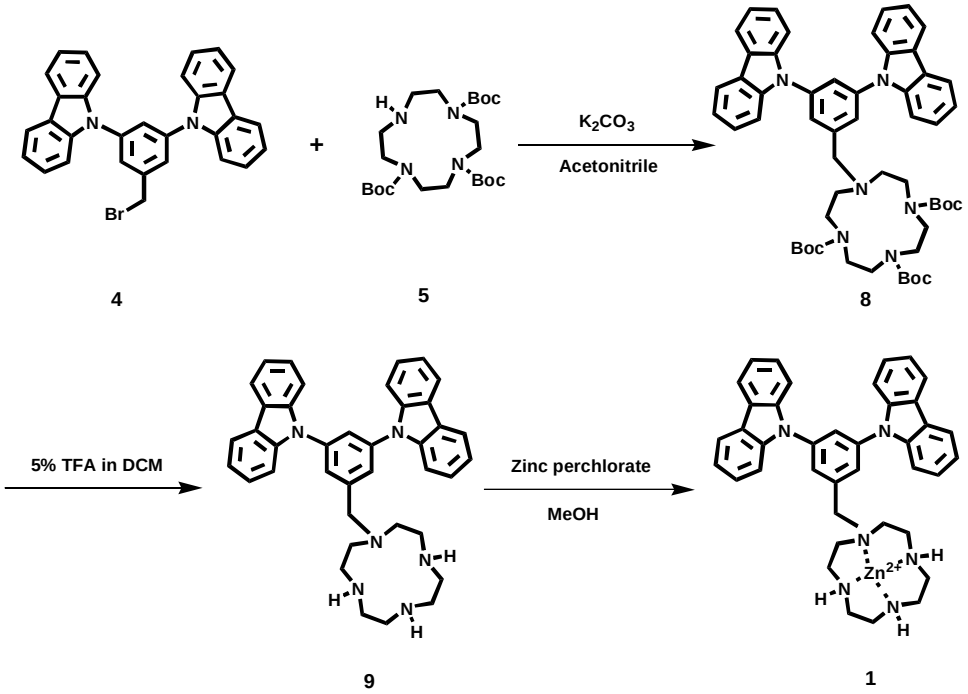
1. Synthesis

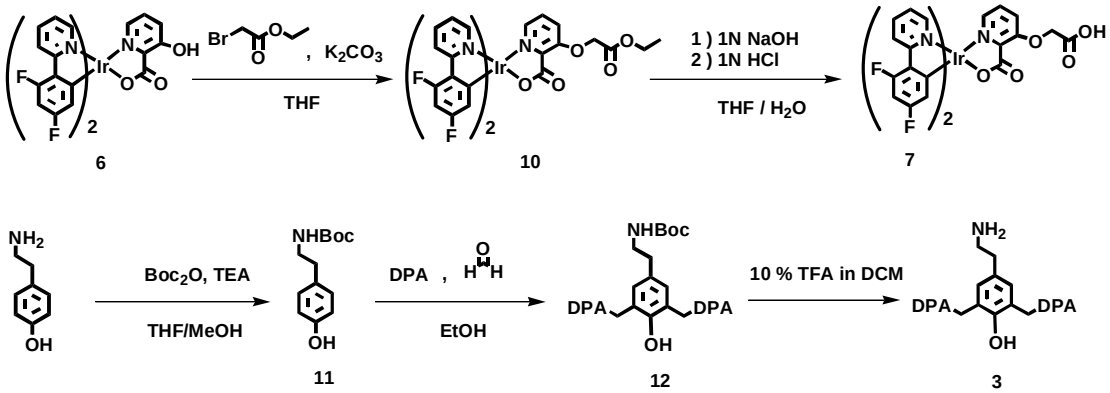
Scheme S1. Synthesis of compound **4**.

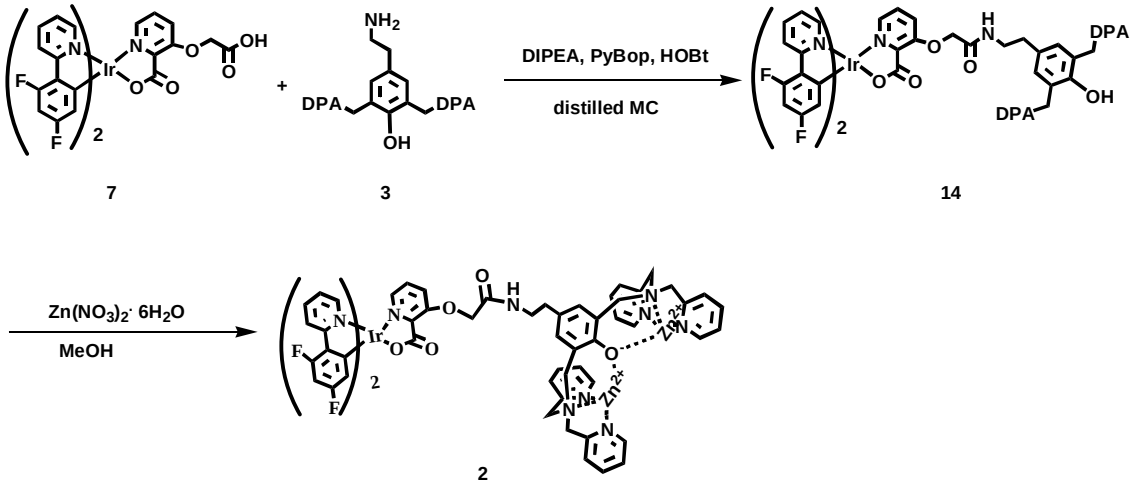


Scheme S2. Synthesis of mCPZnCy (**1**).



Scheme S3. Synthesis of FIrpicZnDPA (**2**).





7 3 14 2

2. Job plot

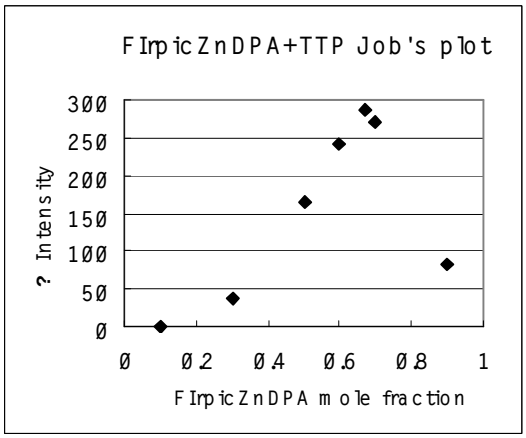


Figure S1. The Job plot between FIrpicZnDPA (**2**) and TTP in 10 mM HEPES buffer at 298 K and pH 7.4. The total concentration of the two compounds is 50 μM.

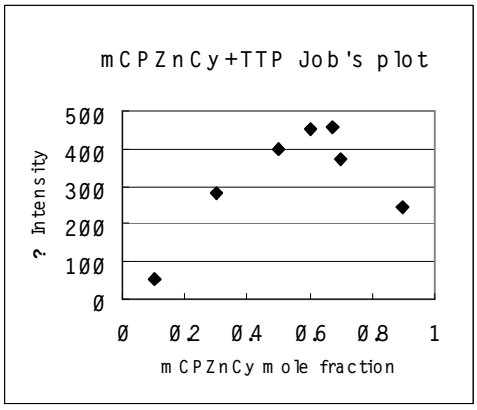


Figure S2. The Job plot between mCPZnCy (**1**) and TTP in 10 mM HEPES buffer at 298 K and pH 7.4. The total concentration of the two compounds is 50 μM.

3. PL Spectra

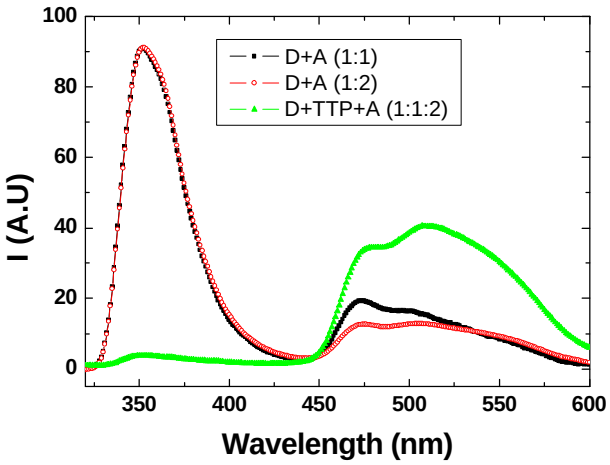


Figure S3. PL spectra in HEPES buffer at 298 K and pH 7.4 upon excitation at 310 nm. (black) **1** (10 μM) + **2** (10 μM), (red) **1** (10 μM) + **2** (20 μM), and (green) **1** (10 µM) + **2** (20 μM) + TTP (10 μM).

Without TTP, the acceptor (**2**) emission intensity is similar, irrespective of the concentration of the acceptor (**2**) when excited at the donor (**1**) absorption peak (λ_{ex} = 310 nm). This is because the distance between the donor and the acceptor is too far away for the efficient intermolecular energy transfer in the mixture of the donor and the acceptor. However, with TTP, the acceptor emission intensity increases more than three times compared with that without TTP due to the intermolecular energy transfer in the 1:1:1 termolecular complex.

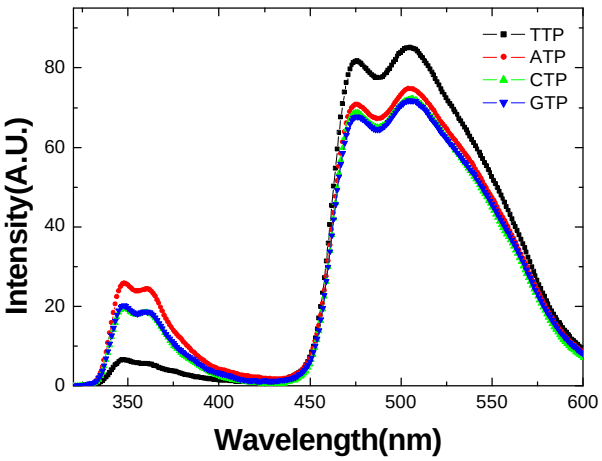


Figure S4. Photoluminescence spectra of **1** (10 μM) + nucleotides (TTP, ATP, CTP, GTP) (each 10 μM) + **2** (20 μM) in HEPES buffer at 298 K and pH 7.4, upon excitation at 310 nm.

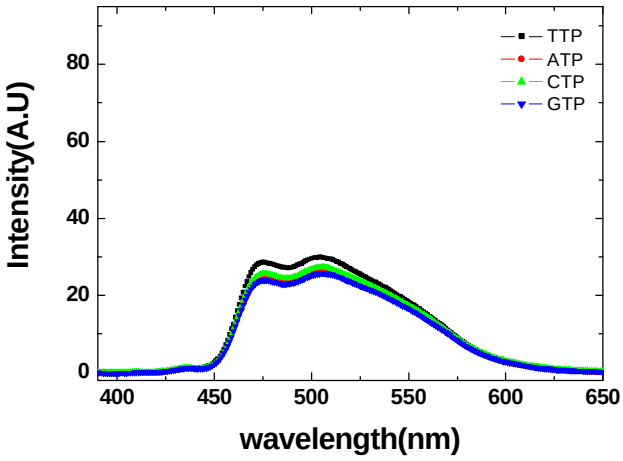


Figure S5. Photoluminescence spectra of **1** (10 μM) + nucleotides (TTP, ATP, CTP, GTP) (each 10 μM) + **2** (20 μM) in HEPES buffer at 298K and pH 7.4, upon excitation at 380 nm.

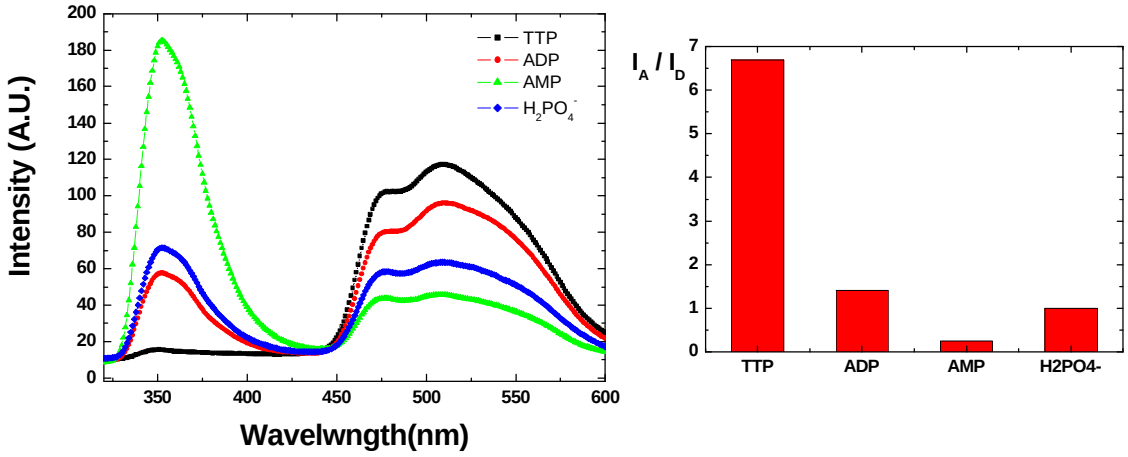
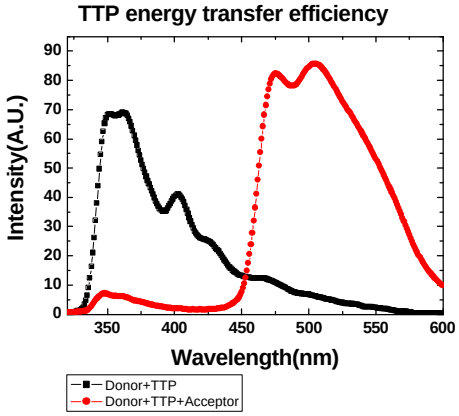


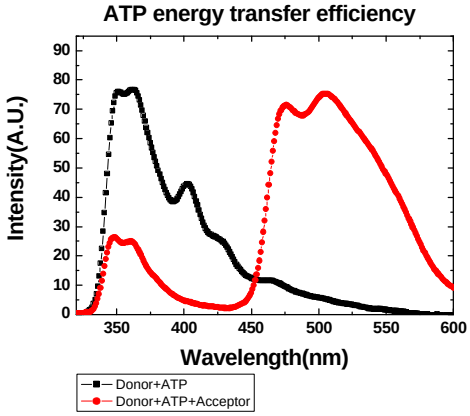
Figure S6. Photoluminescence spectra of **1** (10 μM) + various anions (TTP, ADP, AMP, $H_2PO_4^-$) (each 10 μM) + **2** (20 μM) in HEPES buffer at 298 K and pH 7.4, upon excitation at 310 nm. The right box shows the relative ratios when the acceptor emission intensity (I_A) at 476 nm is divided by the residual donor emission (I_D) at 348 nm.

4. Energy Transfer (ET) Efficiency via Steady-State PL method

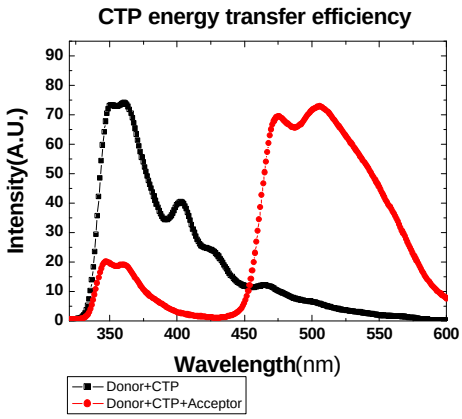
In the steady state PL method, ET efficiency was measured from the extent of the luminescence quenching of the donor in the presence of the acceptor. This was measured from the relative ratio between the integrated area of the donor peak in the **1** + TTP (IA_{D+T}) and that of the donor peak in **1** + TTP + **2** (IA_{D+T+A}). The ET efficiency was (1 - IA_{D+T+A}/IA_{D+T}) × 100 (%). All the measurements were done in an aqueous solvent of HEPES buffer (10 mM, pH 7.4) at 25? .



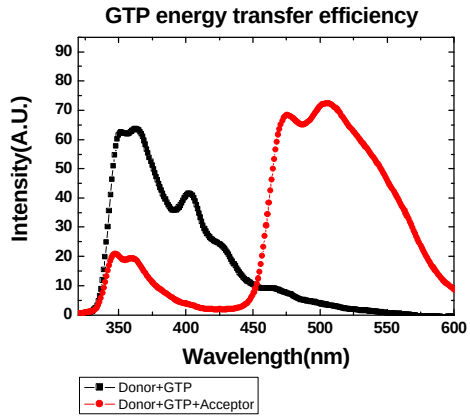
ET = 91%



ET = 74%



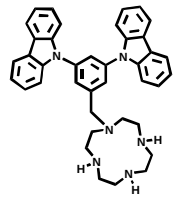
ET = 79%



ET = 76%

Figure S7. PL spectra of **1** (10 μM) + NTP (10 μM) and **1** (10 μM) + NTP (10 μM) + **2** (20 μM). ET efficiency was measured according to the above equation.

NMR Spectra



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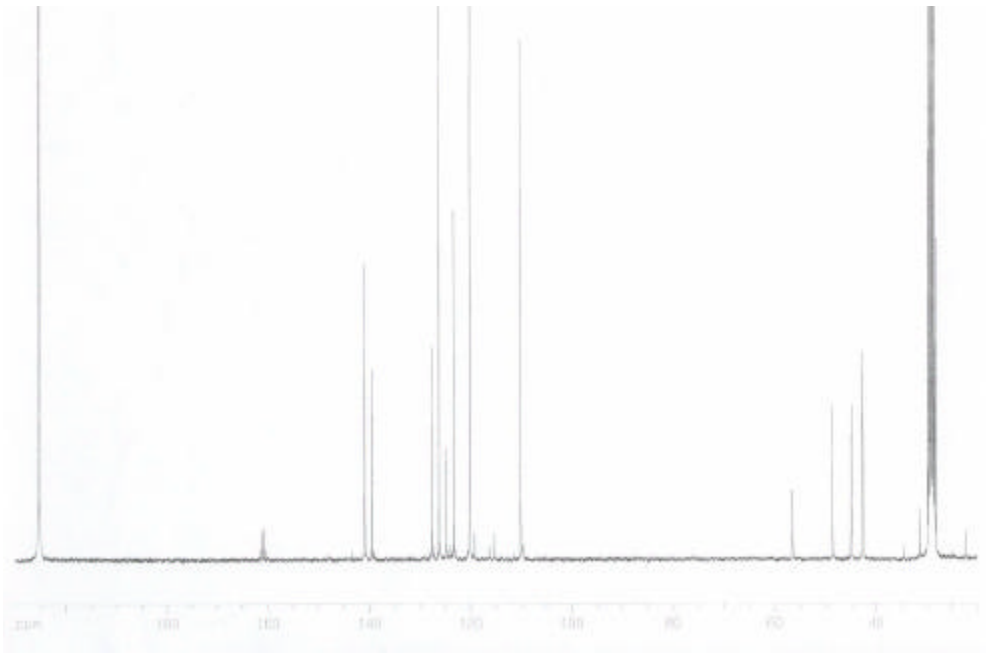

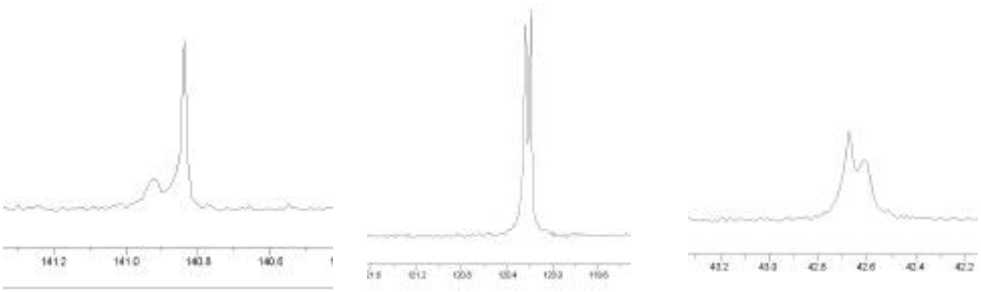

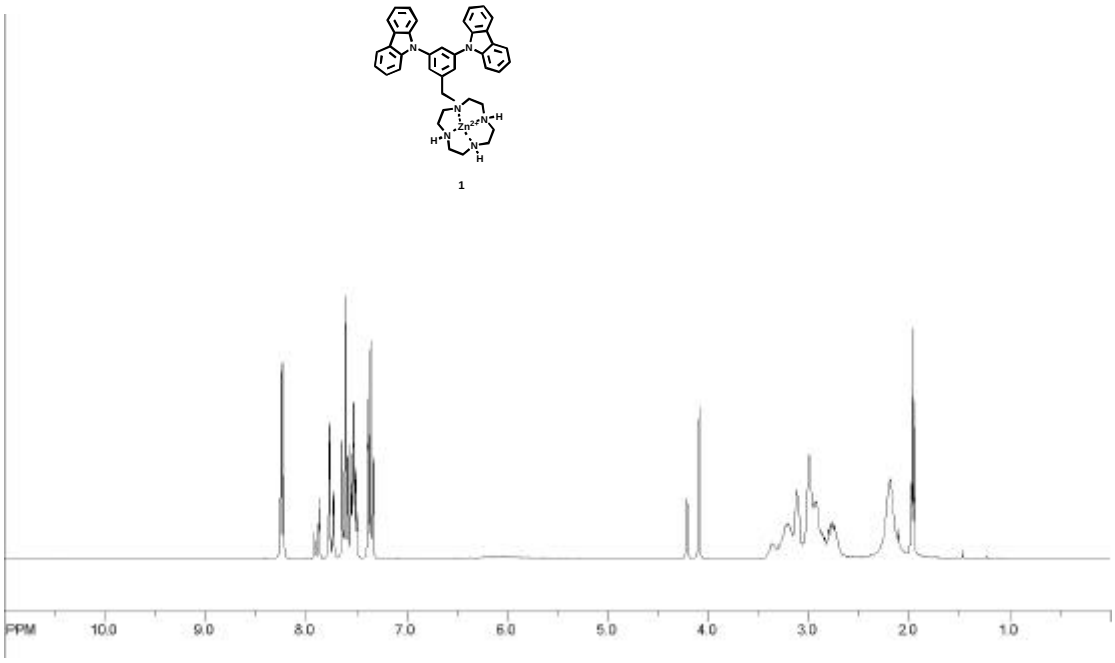

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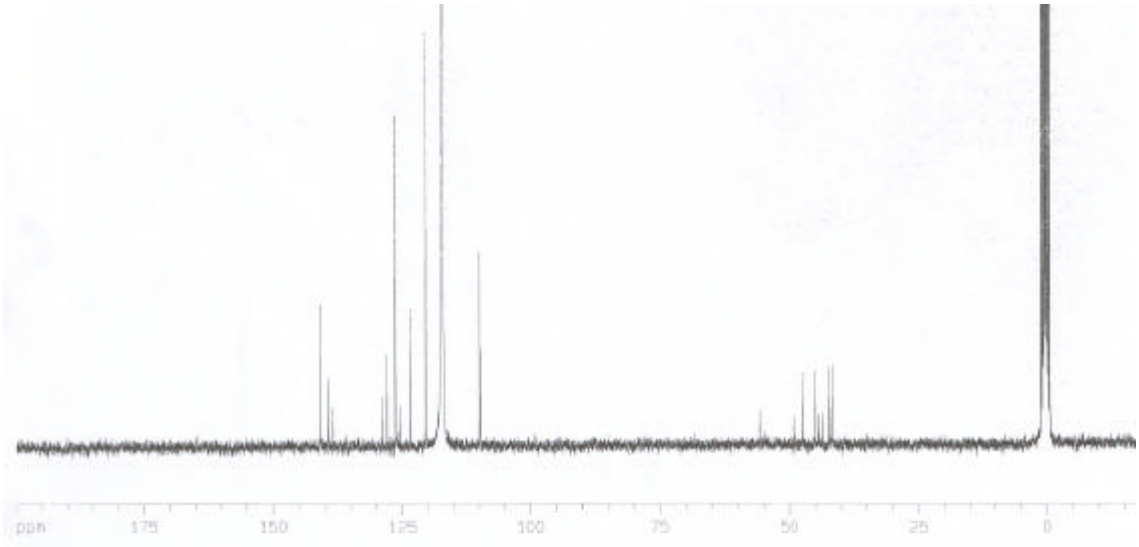

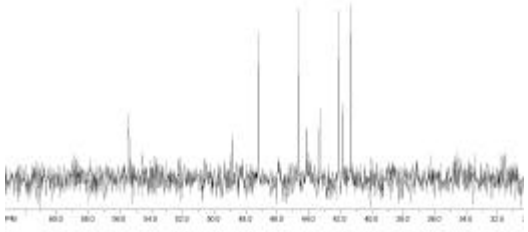

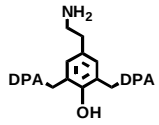
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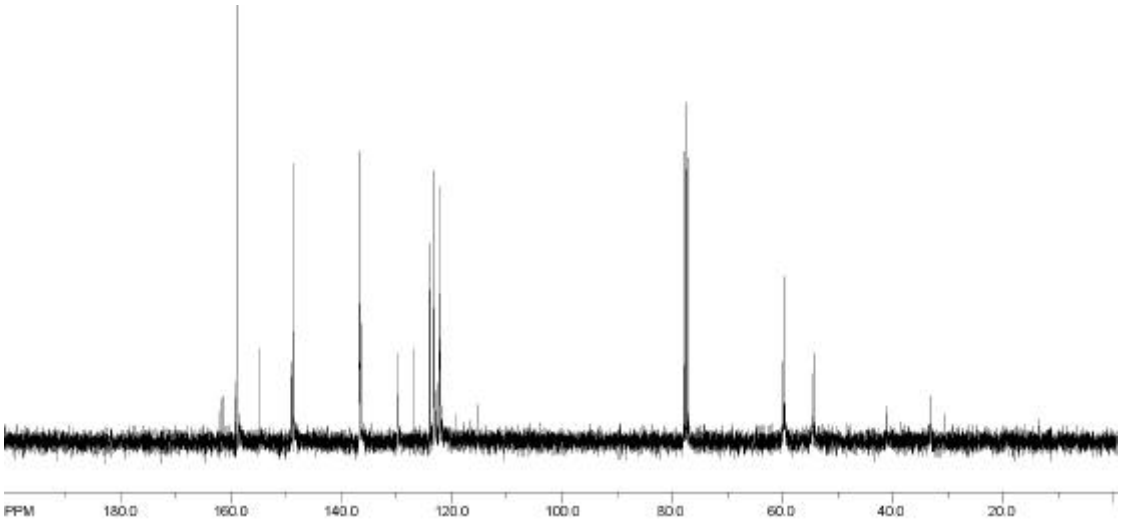
1.0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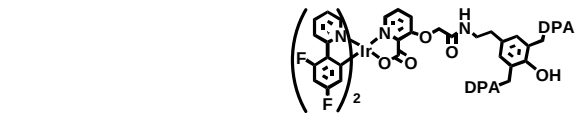
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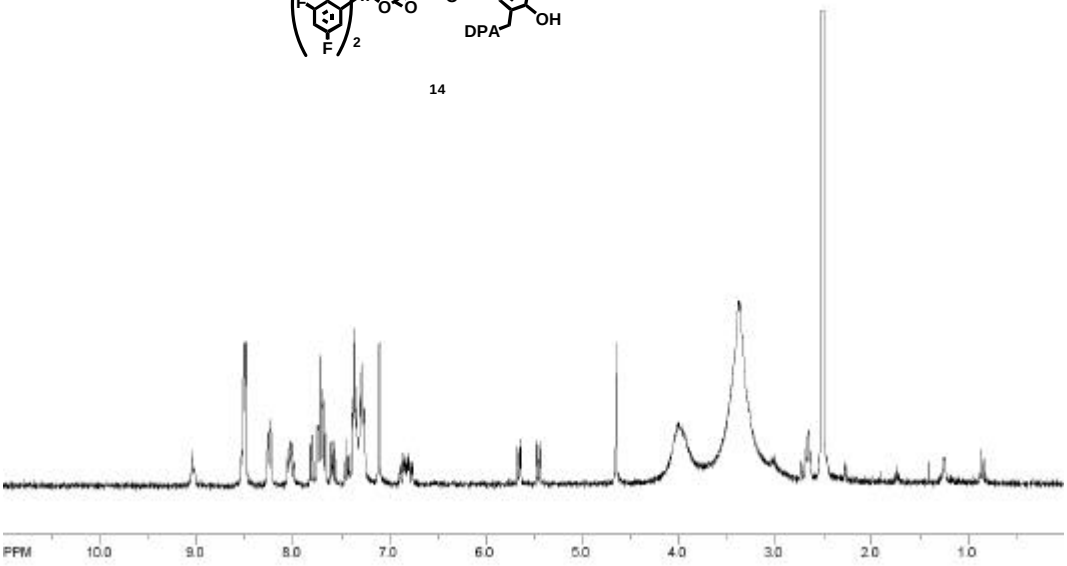
OH

14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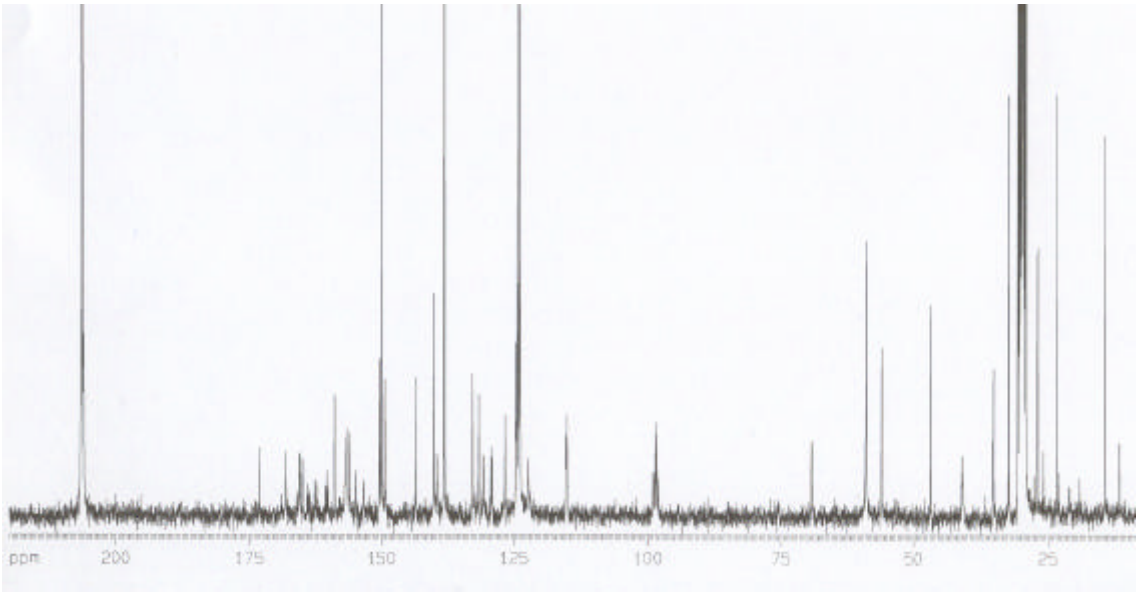
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