Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Exploring the role of the 5-substituent for the intrinsic fluorescence of 5-aryl and 5-heteroaryl uracil nucleotides: A systematic study

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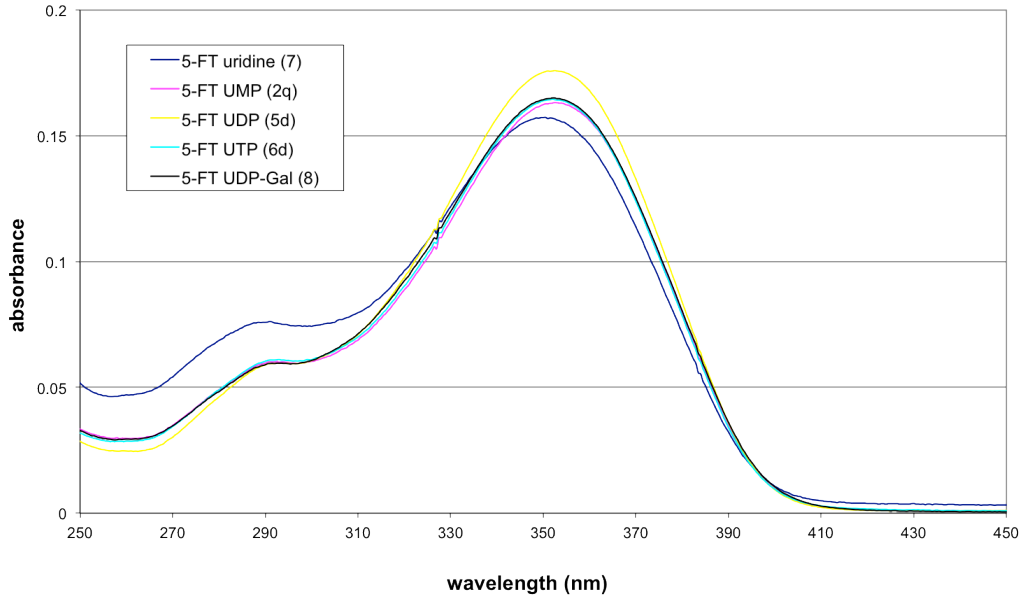
(1) Additional figures

Figure S1. Absorbance (top) and fluorescence (bottom) spectra for different 5-(5-formylthien-2-yl)-substituted uracil fluorophores in water (at 1 μM).



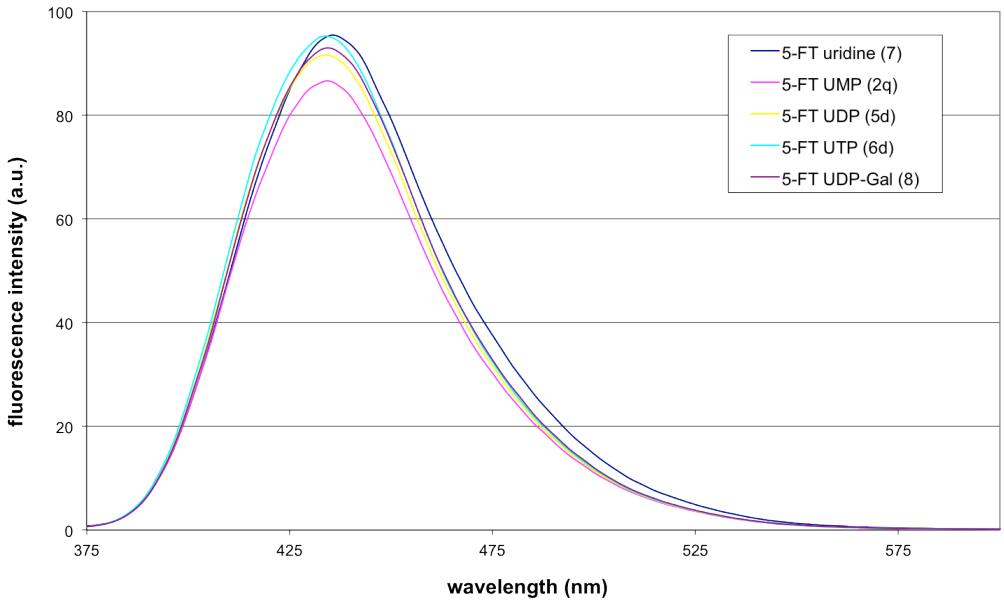


Figure S2. Calculated and experimental absorbance spectra for UMP derivatives **2m**, **2n**, **2p** and **2q**.

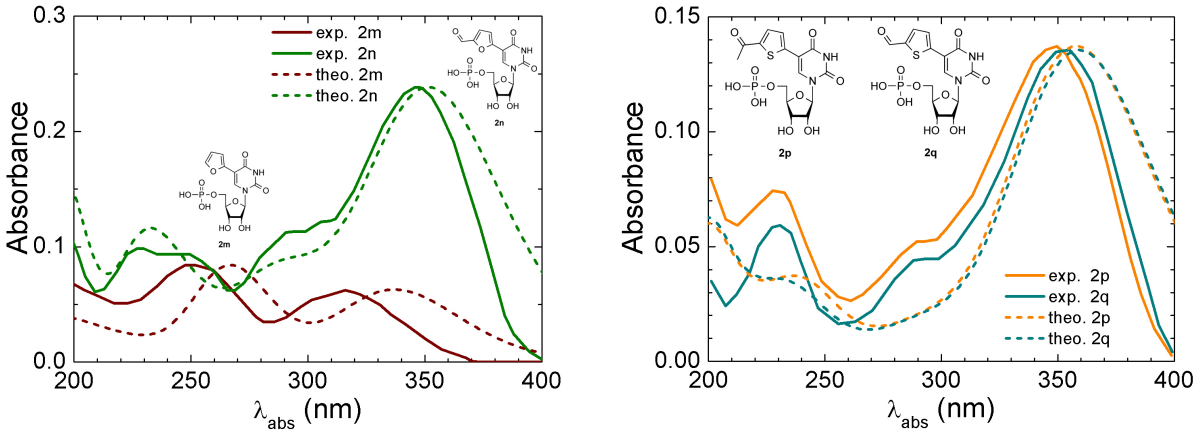
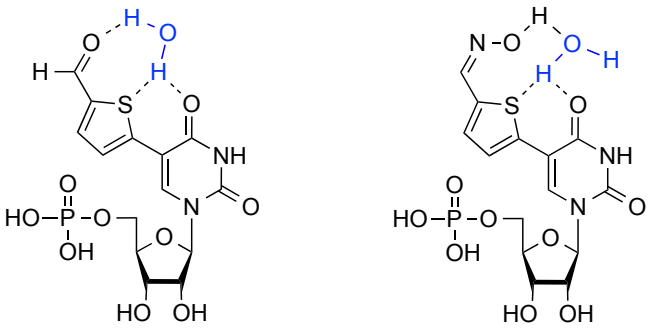


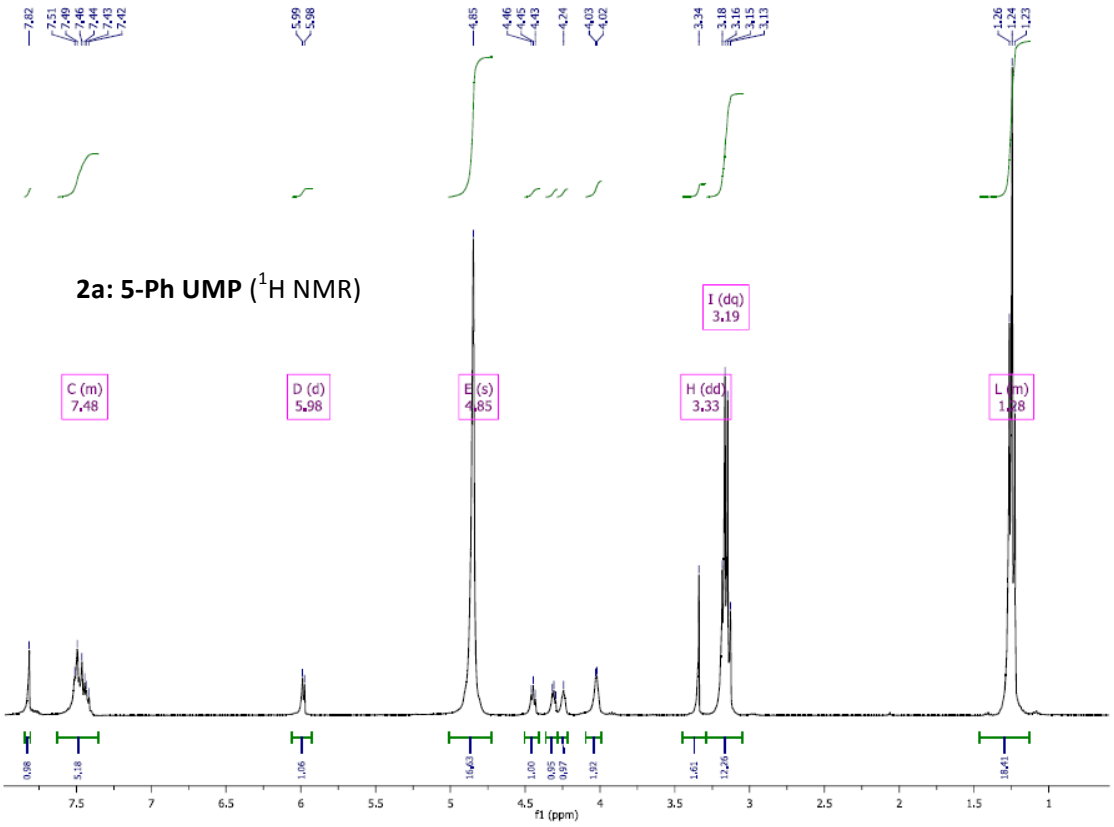
Figure S3. Potential stabilization of the coplanar, fluorescent conformation of **2q** and *anti*-**2r** through putative hydrogen bonding.



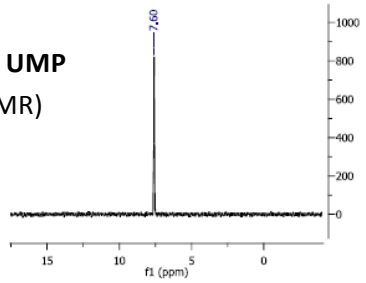
2q *anti*-**2r**

(2) NMR spectra of compounds 2a, 2b and 2l-q

2a: 5-Ph UMP (^{1}H NMR)



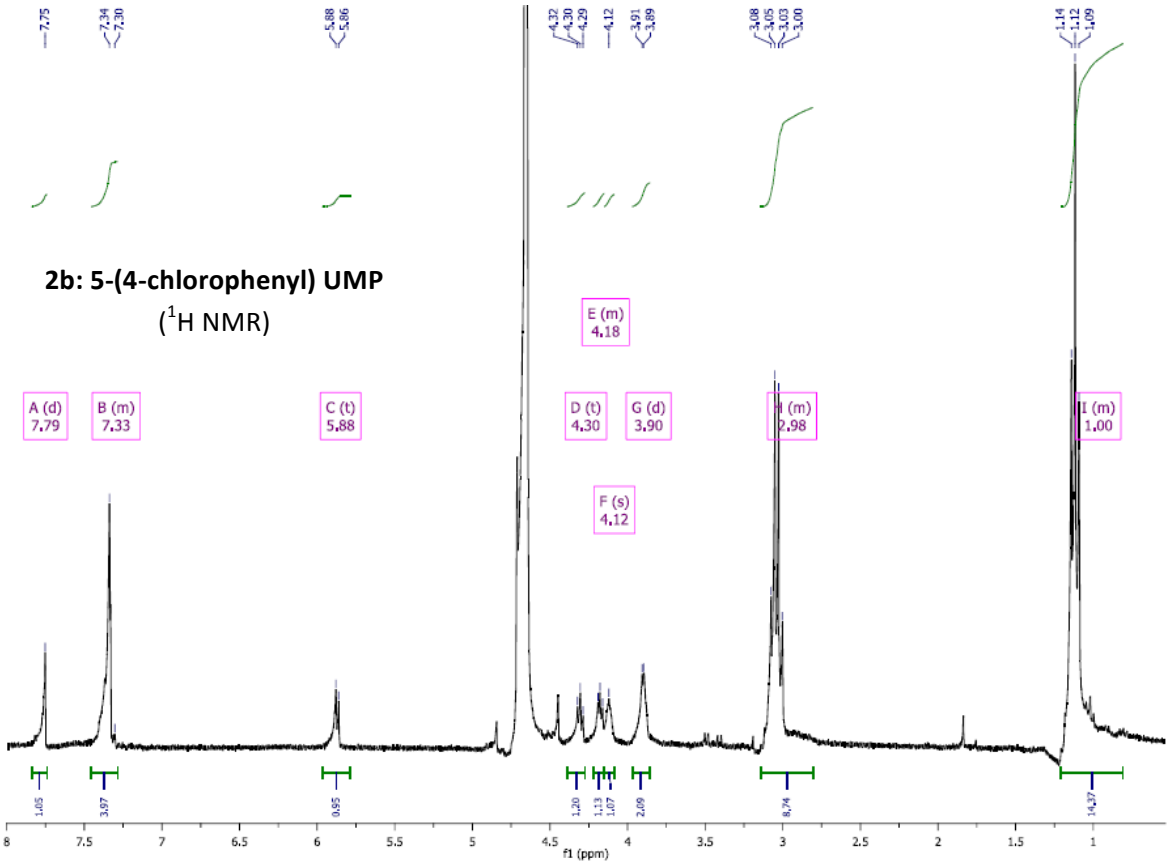
2a: 5-Ph UMP
(^{31}P NMR)



2a: 5-Ph UMP (^{13}C NMR)

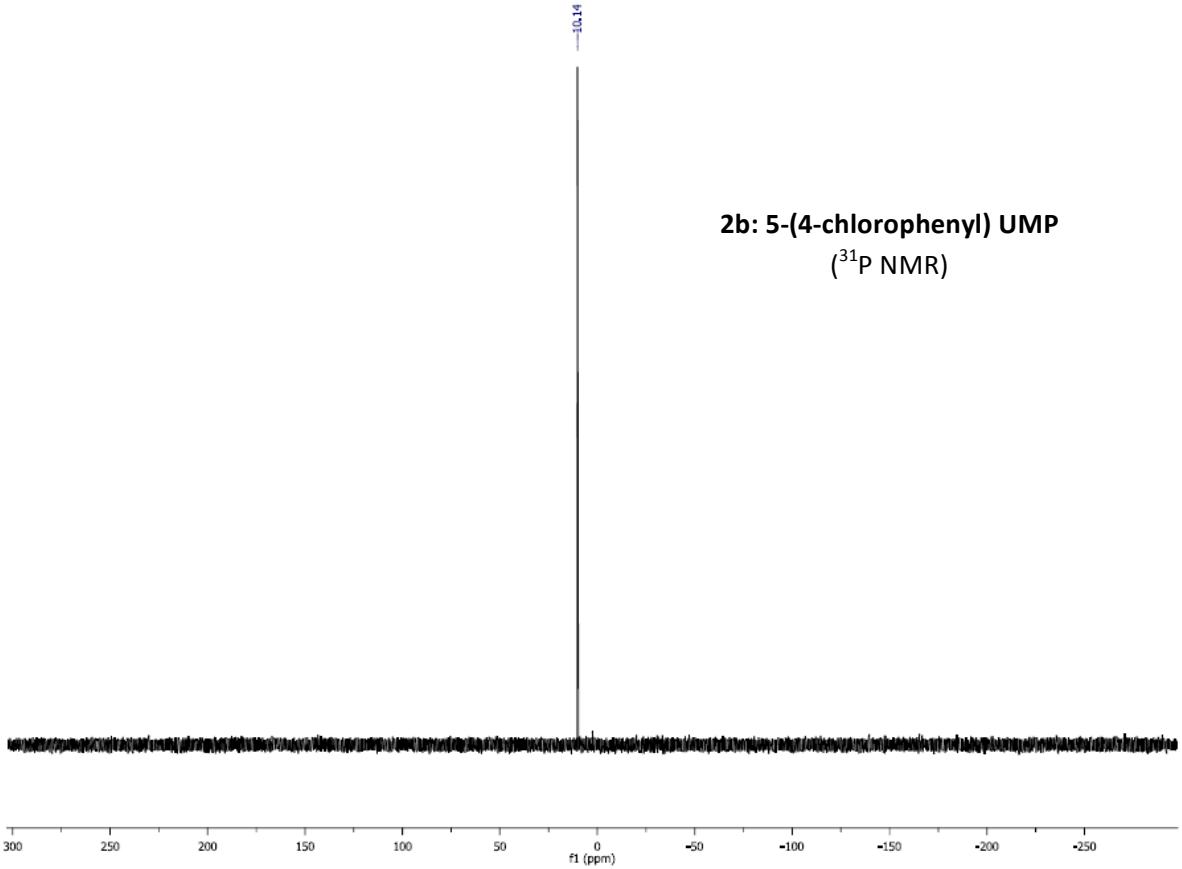
2b: 5-(4-chlorophenyl) UMP

(^{1}H NMR)

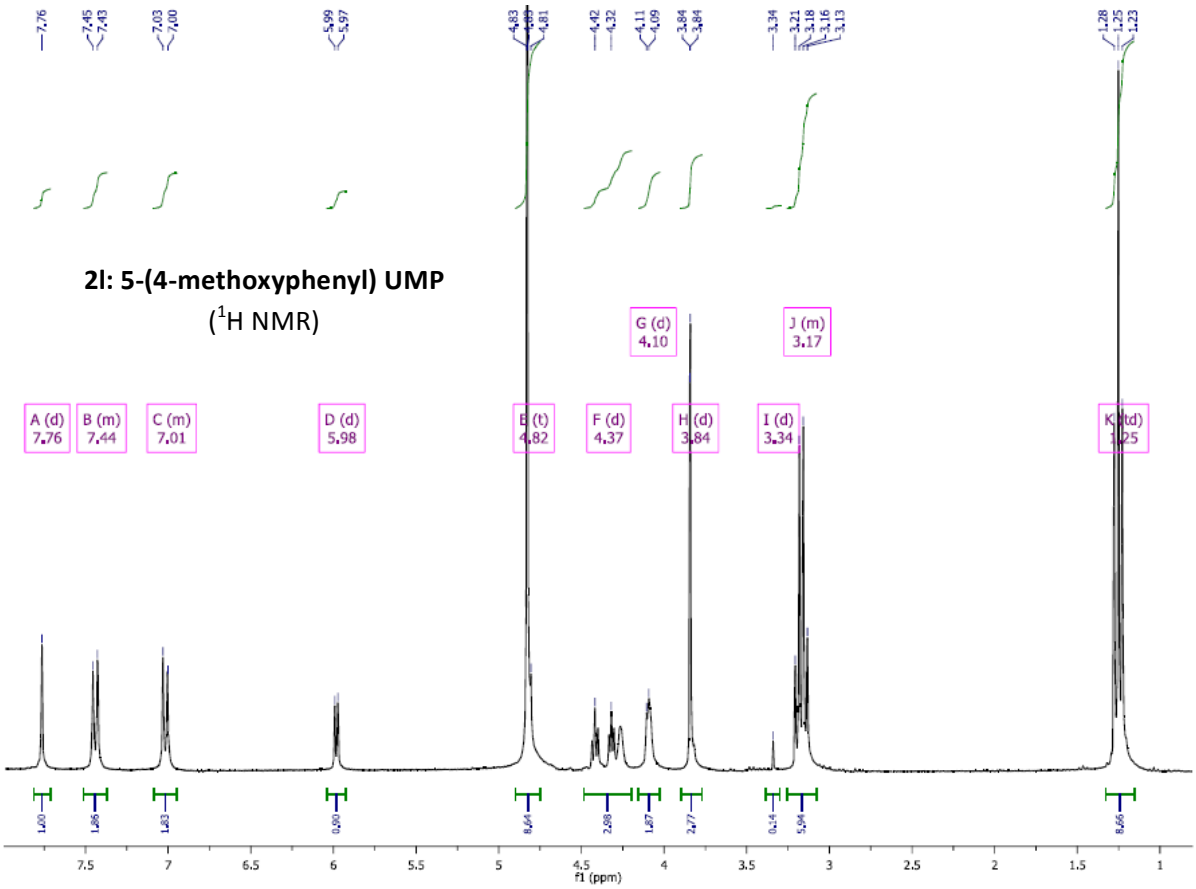


2b: 5-(4-chlorophenyl) UMP

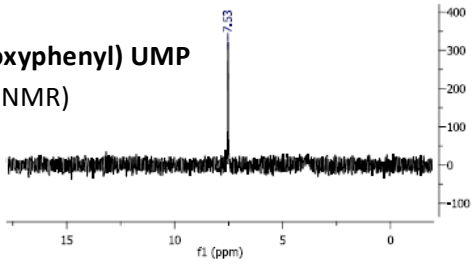
(^{31}P NMR)



2l: 5-(4-methoxyphenyl) UMP
(^{1}H NMR)

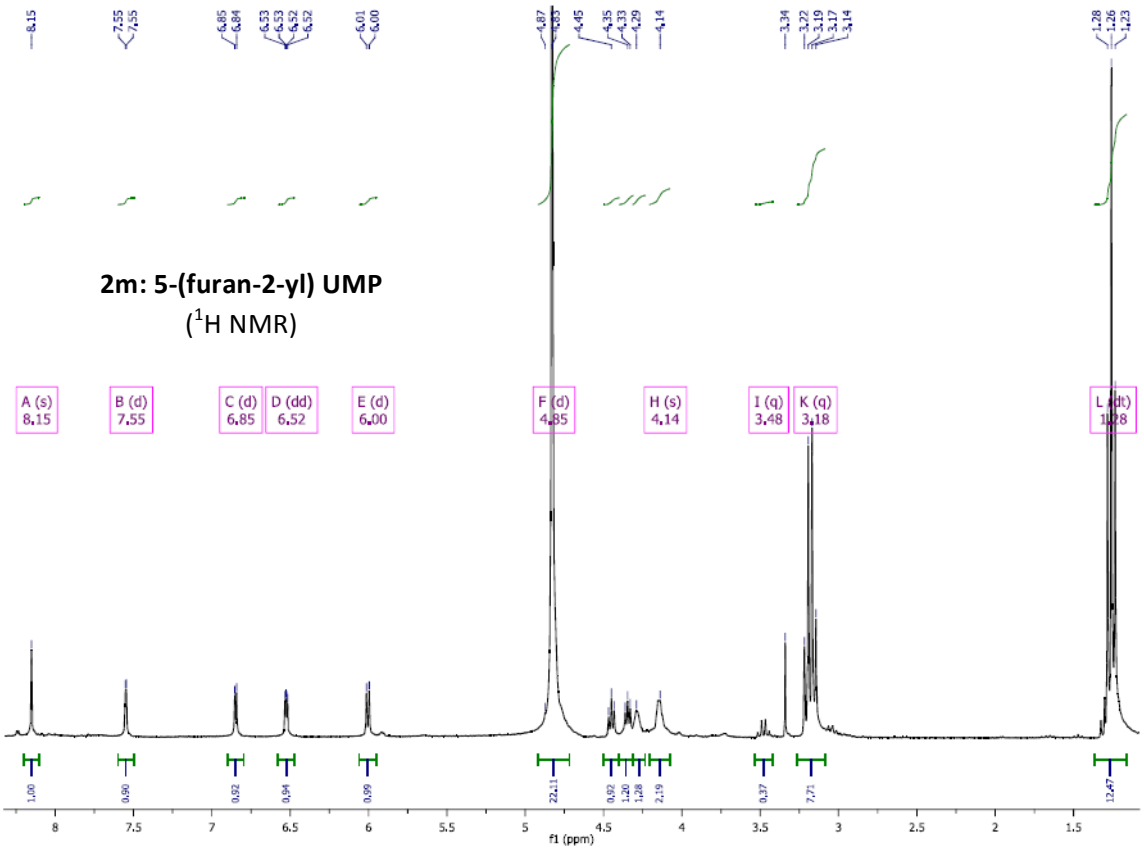


2l: 5-(4-methoxyphenyl) UMP
(^{31}P NMR)

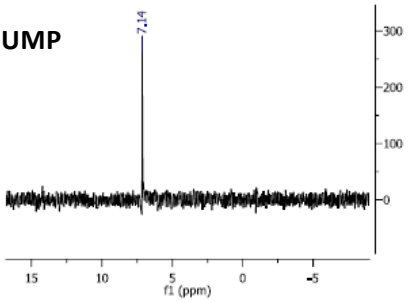


2l: 5-(4-methoxyphenyl) UMP
(^{13}C NMR)

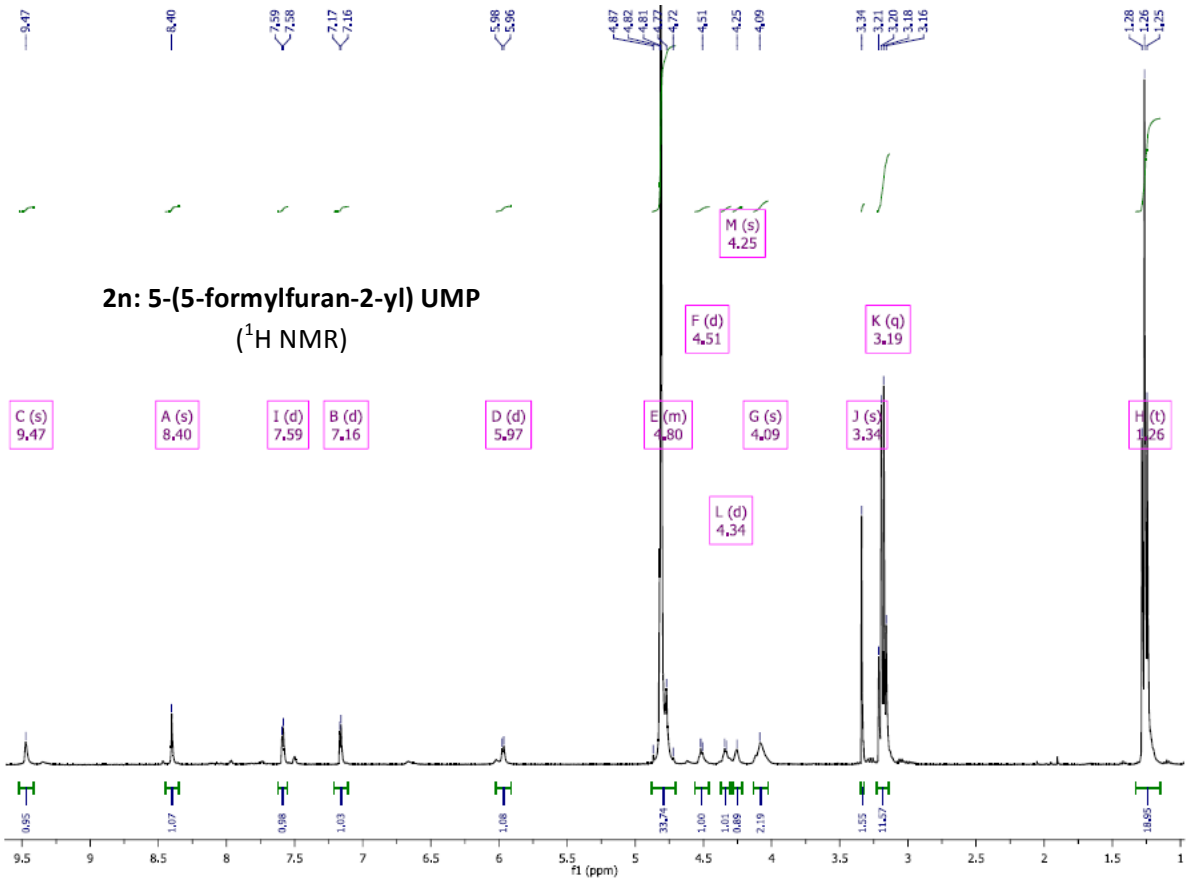
2m: 5-(furan-2-yl) UMP
(^{1}H NMR)



2m: 5-(furan-2-yl) UMP
(^{31}P NMR)

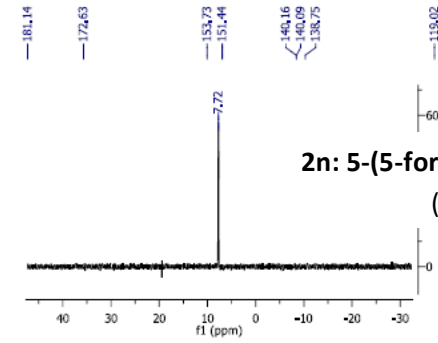


2m: 5-(furan-2-yl) UMP
(^{13}C NMR)



2n: 5-(5-formylfuran-2-yl) UMP

(^{1}H NMR)



2n: 5-(5-formylfuran-2-yl) UMP

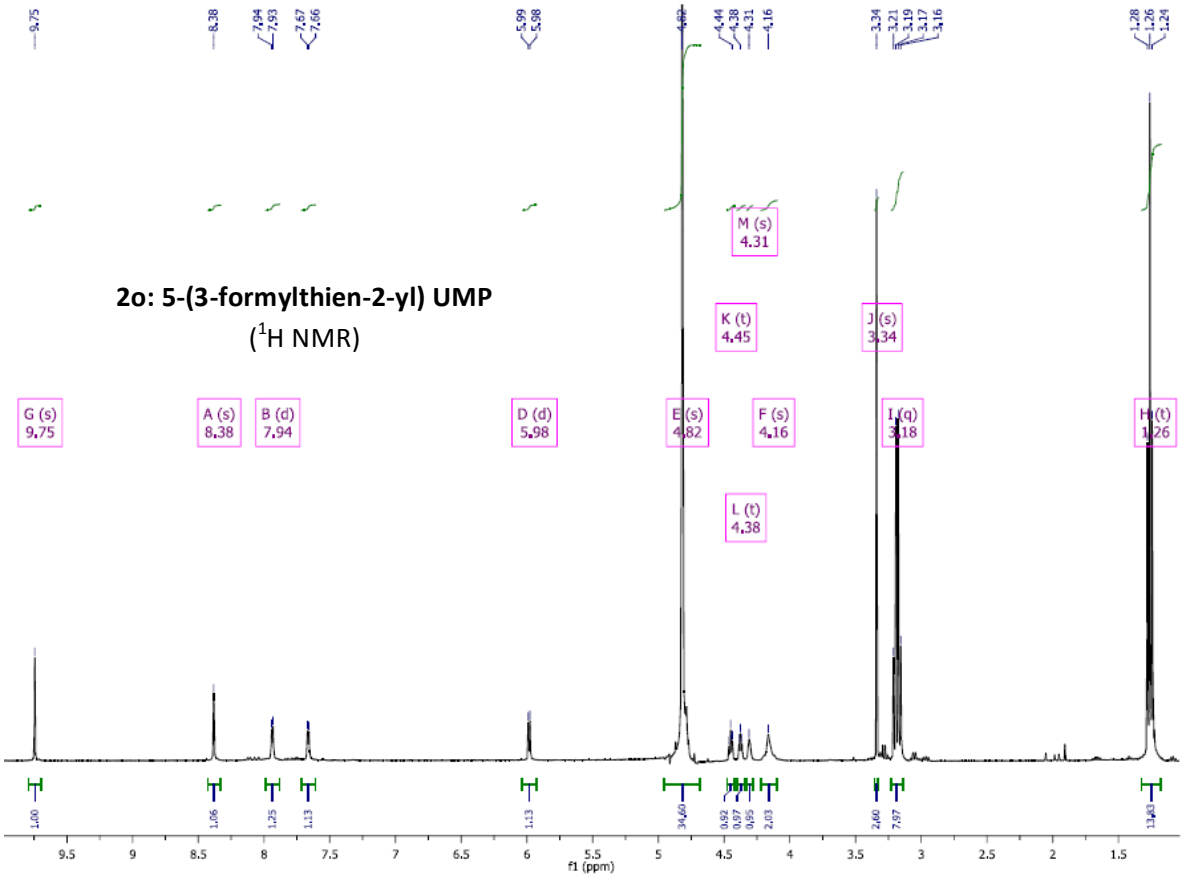
(^{31}P NMR)

2n: 5-(5-formylfuran-2-yl) UMP

(^{13}C NMR)

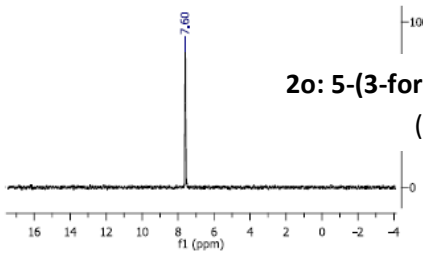
2o: 5-(3-formylthien-2-yl) UMP

(^{1}H NMR)



2o: 5-(3-formylthien-2-yl) UMP

(^{31}P NMR)

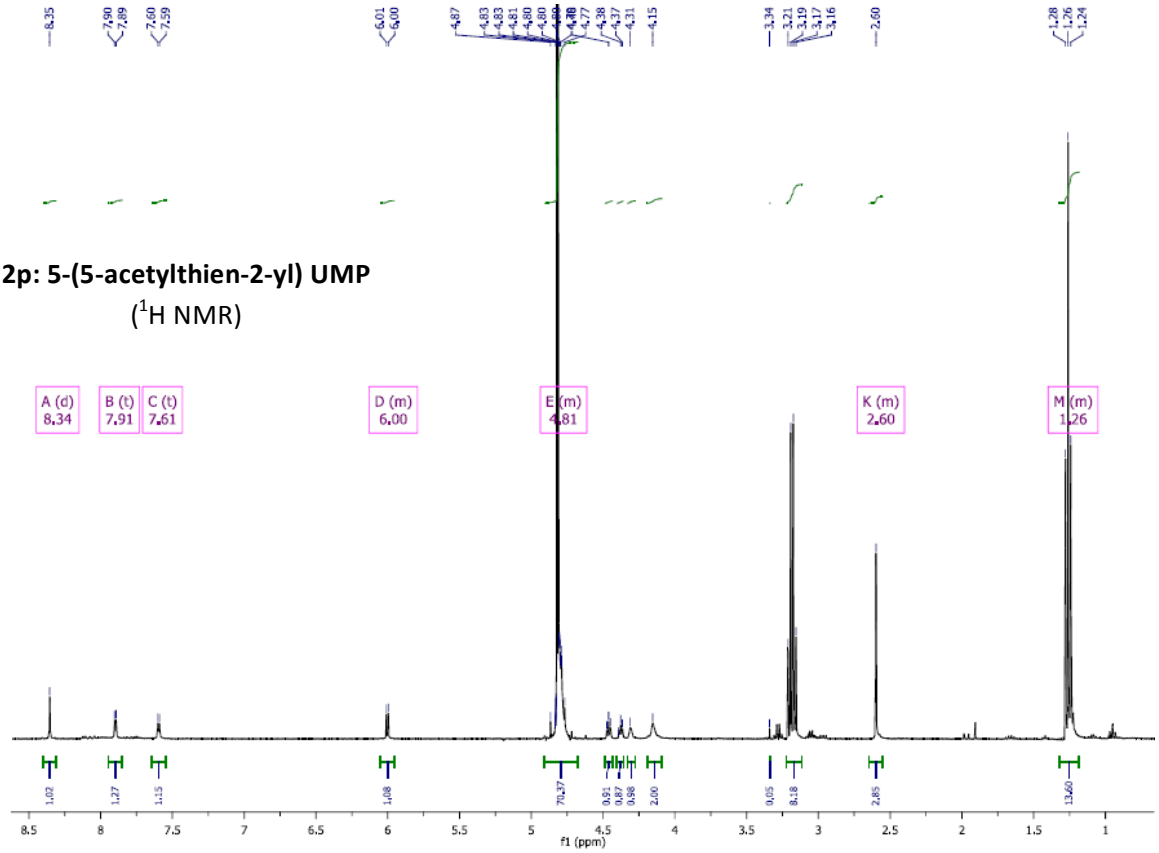


2o: 5-(3-formylthien-2-yl) UMP

(^{13}C NMR)

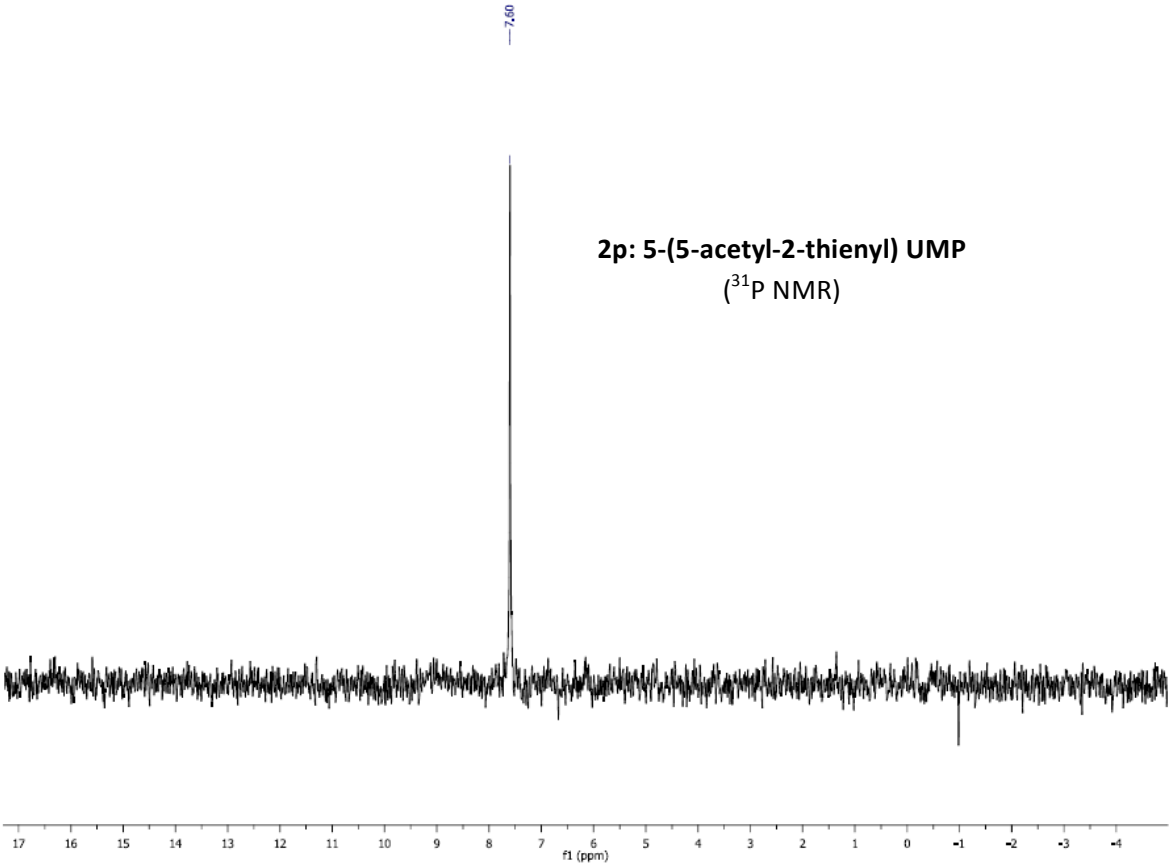
2p: 5-(5-acetylthien-2-yl) UMP

(^{1}H NMR)



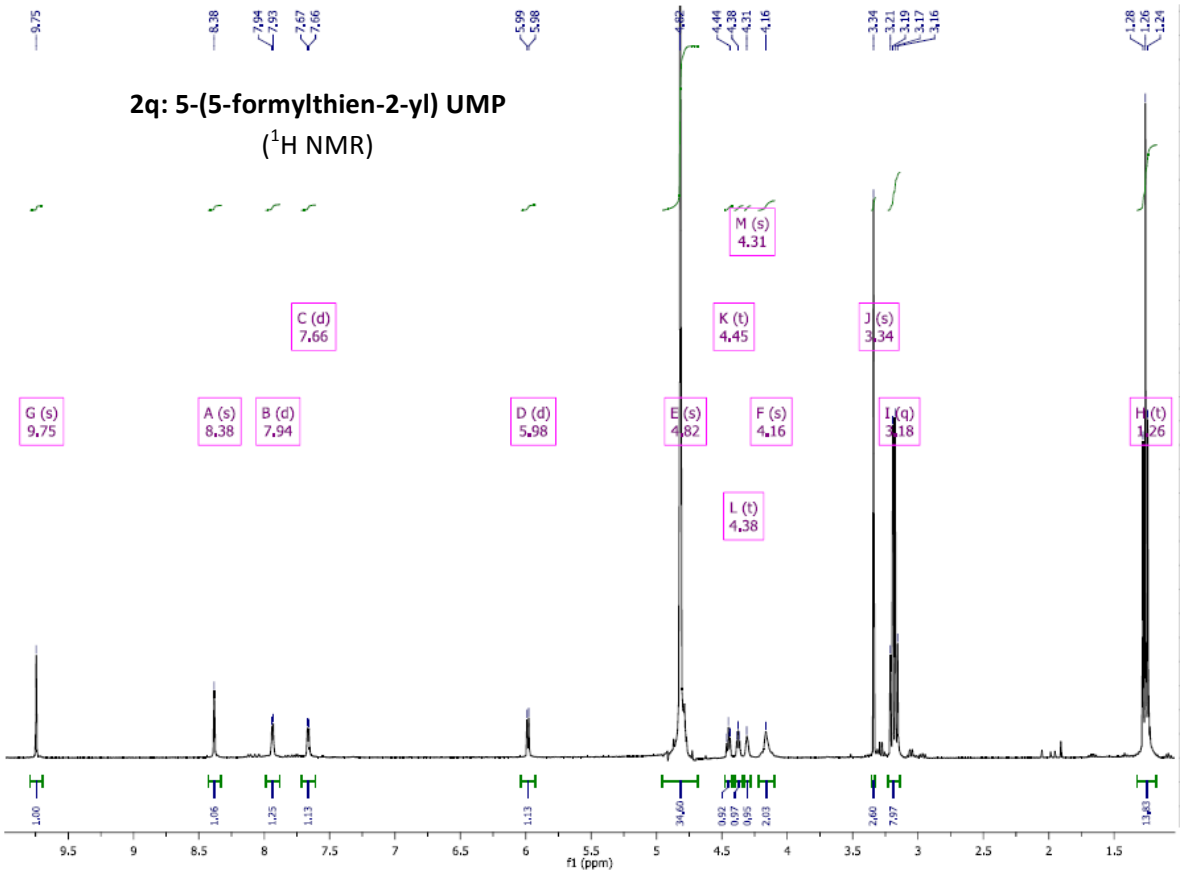
2p: 5-(5-acetyl-2-thienyl) UMP

(^{31}P NMR)



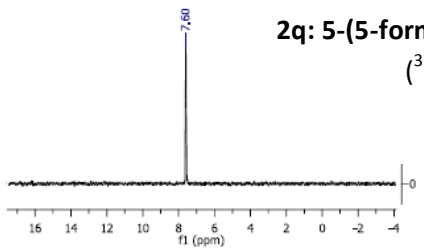
2q: 5-(5-formylthien-2-yl) UMP

(^{1}H NMR)



2q: 5-(5-formylthien-2-yl) UMP

(^{31}P NMR)



2q: 5-(5-formylthien-2-yl) UMP

(^{13}C NMR)