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Supporting Information

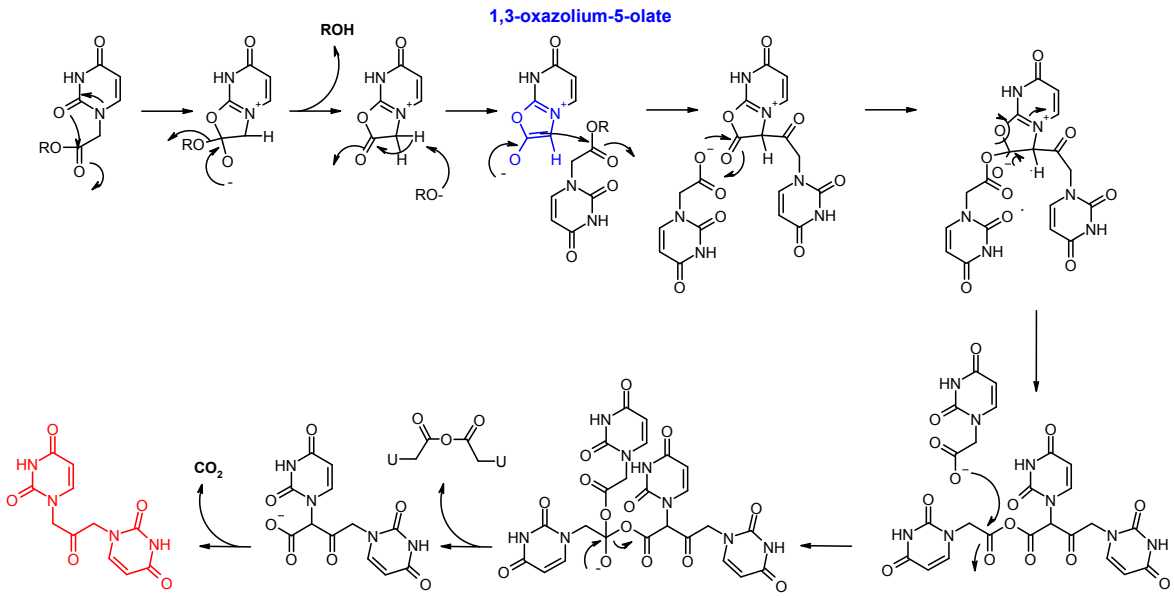
Synthesis and supramolecular assembly of 1,3-bis(1'-uracilyl)-2-propanone

Giovanni N. Roviello[a]*, Giuseppina Roviello[b], Domenica Musumeci[c], Domenica Capasso[d], Sonia Di Gaetano [a], Michele Costanzo[d], Carlo Pedone[d]

[a]Dr. G. N. Roviello, Dr. S. Di Gaetano
Istituto di Biostrutture e Bioimmagini – CNR, Via Mezzocannone 16, 80134 Napoli, Italy;
[b]Dr. G. Roviello
Department of Science and Technology, University of Naples "Parthenope", Centro Direzionale, 80143 Napoli, Italy;
[c]Dr. D. Musumeci
Department of Chemical Science, University of Naples "Federico II", Via Cinthia, 80126 Napoli, Italy;
[d]Dr. D. Capasso, M. Costanzo, Prof. C. Pedone
Department of Pharmacy, University of Naples "Federico II", Via Mezzocannone 16, 80134, Napoli, Italy.

Mechanicistic considerations

Mechanism for the reaction performed with the above procedure can be interpretated as depicted in Scheme S1 and involves the formation of a 1,3-oxazolium-5-olate intermediate obtained after cyclodehydratation of the HATU-activated uracilyl acetic acid derivative (UCH_2COOR).



Scheme S1. Mechanism for the reaction that leads to U_2CO.

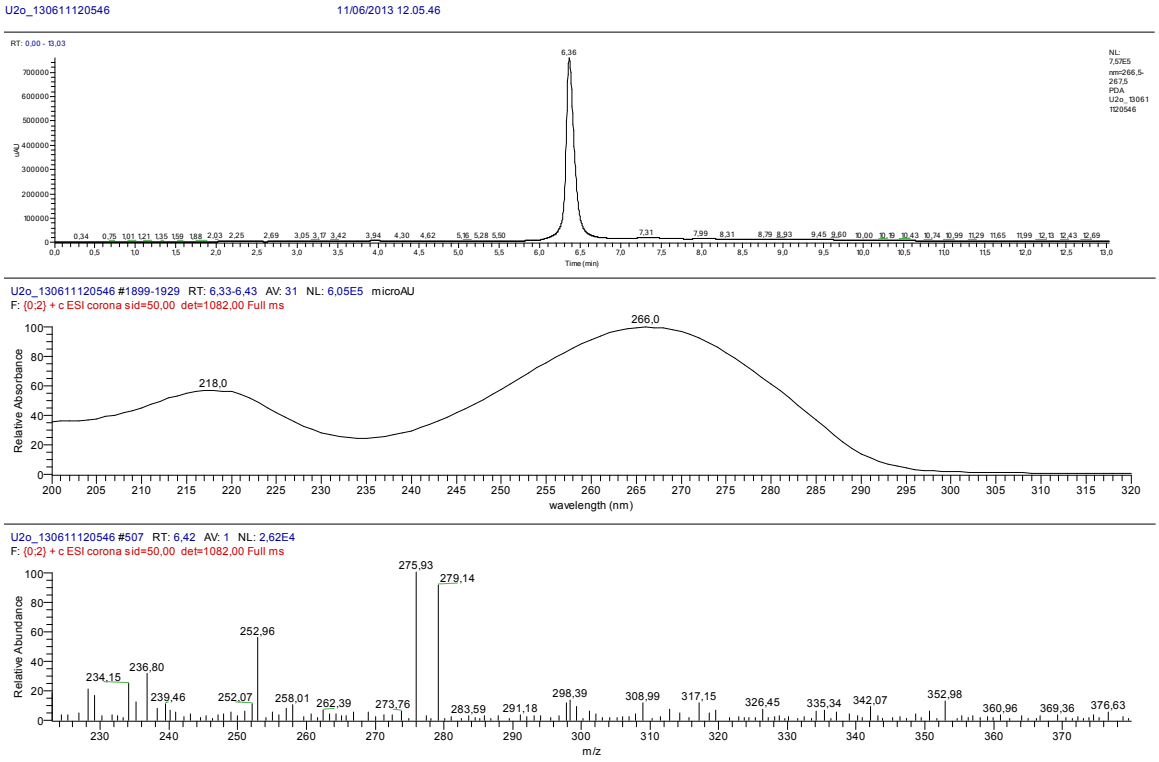


Fig. S1 LC ESI MS (positive ions) of U_2CO. Analytical HPLC was obtained by a C_{18} column (Phenomenex Jupiter C18 300 Å, 5 µm, 4.6×150 mm) with a flow rate of 0.8 mL/min and a linear gradient from 2% (for 5 min) to 30% B in A over 10 min: t_R=6.4 min (A = 0.1% TFA in water; B = 0.1% TFA in acetonitrile).

Table S1. Crystallographic data for U_2CO

	U_2CO
Chemical formula	$C_{11}\ H_{10}\ N_4\ O_5$
Crystal size, mm	0.15× 0.10 × 0.10
Crystal habitus, colour	Prism, white
Formula weight	278.23
Temperature (K)	173
λ (Å)	0.71069
Crystal system	monoclinic
Space group	*P2/c*
a (Å)	15.061(1)
b (Å)	4.938(2)
c (Å)	20.805(2)
α (°)	90
β (°)	130.93(1)
γ (°)	90
Volume ($Å^3$)	1168.9
Z	4
D_{calcd} ($g \cdot cm^{-3}$)	1.581
μ (mm^{-1})	0.128
F(000)	576
Theta range (°)	3.58, 27.50
Reflections collected	11761
Unique observed reflections	2645 [R(int) = 0.0757]
Data/parameters	2645/185
R1[a], wR2[b] [I>2σ(I)]	0.0710, 0.2209
R1[a], wR2[b] (all data)	0.1173, 0.2947
Largest diff. peak and hole ($e \cdot Å^{-3}$)	0.426, -539

[a] $R_1 = \Sigma||Fo|-|Fc|/\Sigma|Fo|$.

[b] $wR_2 = [\Sigma w(Fo^2-Fc^2)^2/\Sigma w(Fo^2)^2]^{1/2}$

Table S2. Recorded values of hydrodynamic diameter with the corresponding standard deviations (sd) relative to different concentrations of U_2CO.

Conc. (μM)	d_h (nm)	sd (nm)
129.0	192.8	43.7
115.4	198.6	77.6
104.4	200.3	85.3
95.3	208.0	83.8
87.7	252.0	98.3
81.2	246.4	92.2
75.6	217.2	94.9
64.5	287.5	104.3