# Electronic supplementary materials

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## Polyether-functionalised uridine as an ion receptor

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### Materials and Methods

The ESI (electro spray ionization) mass spectra were recorded on a Waters/Micromass (Manchester, UK) ZQ mass spectrometer equipped with a Harvard Apparatus syringe pump. The measurements were performed for two types of samples: acetonitrile solutions of **3** or **5** ($1\times10^{-3}$ mol dm$^{-1}$) with a mixture of $Li^+$, $Na^+$, $K^+$, $Rb^+$ and $Cs^+$ cations ($5\times10^{-3}$ mol dm$^{-1}$) and acetonitrile solutions of **3** or **5** ($1\times10^{-3}$ mol dm$^{-1}$) with $Li^+$, $Na^+$, $K^+$, $Rb^+$ and $Cs^+$ cations ($5\times10^{-3}$ mol dm$^{-1}$) taken separately. The samples were infused into the ESI source using a Harvard pump at a rate 20 μdm$^3$ min$^{-1}$. The ESI source potentials were: capillary 3 kV, lens 0.5 kV, extractor 4 kV, the cone voltage was 30 V. The source temperature was 120°C and the dissolvation temperature was 300°C. Nitrogen was used as a nebulizing and dessolvation gas at a flow rates of 100 and 300 dm$^3$ h$^{-1}$ respectively.

The NMR spectra were recorded in the solvents indicated and TMS as an internal (external in the case of $D_2O$) standard on the Varian Gemini 300 MHz spectrometer. $^{23}$Na NMR measurements in acetonitrile were performed at 298 K on Varian Gemini 300 spectrometer equipped with 5 mm 1HBB direct observing probehead, operating at 79.373 MHz. The 1M solutions of NaCl in $D_2O$ were used as the external standards (0.00 ppm).

Elemental analyses were performed with Elementar Vario EL III instrument.

**1-(4,4'-Dimethoxytrityloxy)-8- tosyloxy-(3,6-dioxaoctane) 1**

Monotosylated triethylene glycol [15] (2.9 g, 9.53 mmole) was evaporated with dry pyridine, dissolved in pyridine (20 ml) and dimethoxytrityl chloride (3.62 g, 10.68 mmole) was added. After 3 hrs at room temperature the solvent was evaporated, viscous residue was dissolved in dichloromethane, washed with $NaHCO_3$ dried with $MgSO_4$ and evaporated. Chromatography on silica gel (dichloromethane with gradually rising addition of ethyl acetate 0 – 5%) gave the desired product **1** as an oil (4.62g, 7.62 mmole, 80%).

$^1$H NMR ($CDCl_3$) 7.8 (d, 2H, J=8.5 Hz, Tos), 7.62 (d, 2H, J=8.5 Hz, Tos), 7.18-7.60 (m, 9H, DMTr), 6.80 (m, 4H, DMTr *o-H*), 4.15 (t, 2H, J=4.5 Hz DMTr-OC*H*$_2$CH$_2$), 3.78 (s, 6H,), 3.70-3.60 (m, 8H –C*H*$_2$C*H*$_2$O-), 3.21 (t, 2H, J=4.5 Hz, CH$_2$C*H*$_2$OTos), 2.41 (s, 3H, Tos C*H*$_3$).

**$N^3$-(3,6-Dioxa-8-dimethoxytrityloxy)octyl-2'-*O*-methyl-5'-*O*-dimethoxytrityluridine 2**

2'-O-methyl-5'-O-dimethoxytrityluridine (300mg, 0.53 mmole) and sodium hydride (60% suspension in mineral oil, 25 mg, 0.6 mmole) in dry DMF (5 ml) was stirred for 45 min. at room temperature, then solution of **1** (350 mg, 0.58 mmole) in DMF (2ml) was added and the mixture was stirred and heated at 100° C for 6 hrs. After cooling, ethyl ether (30 ml) was added and the mixture was washed with $NaHCO_3$, dried with $MgSO_4$, and evaporated. Separation on silica gel column (methylene chloride with gradually rising addition of ethyl acetate 0 – 15%) gave the product **2** as colorless oil (190 mg, 0.2 mmole, 38%).

$^1$H NMR ($CDCl_3$) 8.01 (d, 1H, J=7.6 Hz, H-6), 7.45-7.26(m, 18H, DMTr), 6.83-6.79 (m, 8H, DMTr *o-H*), 5.93 (s, 1H, H1'), 5.30 (m, 1H, H-5), 4.58 (m, 1H, H-3'), 4.16 (m, 2H, DMTr-OC*H*$_2$CH$_2$), 3.98 (m, 1H, H-4'). 3.79 (s, 6H, DMTr OC*H*$_3$), 3.77 (s, 6H, DMTr OC*H*$_3$), 3.76-3.53 (m, 14H, 5'C*H*$_2$, H-2', –C*H*$_2$C*H*$_2$O-, 2'-OC*H*$_3$), 3.21 (m, 2H, N-C*H*$_2$CH$_2$).

**$N^3$-(3,6-Dioxa-8-hydroxy)octyl-2'-*O*-methyluridine 3**

Product **2** (190 mg, 0.2 mmole) was dissolved in 80% acetic acid (10 ml). After 30 min at room temperature the solution was evaporated to dryness, co-evaporated twice with toluene and divided between water (10 ml) and toluene (10 ml). The aqueous phase was separated and evaporated, giving clear oil (65 mg, 84%). Elemental analysis ($C_{15}H_{24}N_2O_9$ ) calc. C 47.89%, H 6.43%, N 7.44%; found C 47.72%, H 6.70%, N 7.32%.

$^1$H NMR ($D_2O$) 7.98 (d, 1H, J=8.2 Hz, H-6), 5.99 (d, 1H, J=3.6Hz, H-1'), 5.94 (d, 1H, J=8.2 Hz, H-5), 4.33 (m, 1H, H-3'), 4.19-4.08(m, 2H, H-4', H-2'), 3.95-3.58 (m, 14H, 5'-C*H*$_2$, H-2', polyether C*H*$_2$), 3.54 (s, 3H, 2'-OC*H*$_3$)

$^{13}$C NMR ($D_2O$) 167.61 (C-4), 154.12 (C-2), 142.32 (C-6), 104.23 (C-5), 91.13 (C-1'), 86.78; 85.56 (C-2', C-4'), 74.46, 72.28, 70.77, 69.77, 63.13, 63.05, 60.98 (C-3',C-5',OC*H*$_3$, polyether except N-CH$_2$), 42.95 (N-C*H*$_2$).

**$O^4$-(3,6-Dioxa-8-trityloxy)octyluridine 4**

2',3',5'-tri-O-acetyl-4-(1,2,4-triazol)-yl-uridine [14] (300 mg, 0.68 mmole) and monotritylated triethylene glycol [16] (600 mg, 1.53 mmole) were dissolved in dioxane (10 ml), DBU (0.5 ml, 509 mg, 3,34 mmole) was added and the mixture heated at 70°C for 12 hrs. TLC (methylene

chloride-methanol 19:1) showed presence of several products (partially deacetylated) and no starting material. Dioxane was evaporated and the residual oil was dissolved in methylene chloride, washed with water, and evaporated and. The residue was deacetylated with satd. methanolic ammonia (30 ml, room temp. overnight). Chromatography (silica gel, methylene chloride with gradually rising conc. of methanol 0-5%) gave the product **4** as slightly yellow oil (270 mg, 0.42 mmole, 62%)

$^1$H NMR ($CDCl_3$) 8.12 (d, 1H, J=7.8 Hz, H-6), 7.50-719 (m, 15H, Tr), 5.98(d, 1H, J=7.8 Hz, H-5), 5.77 (d, 1H, J=3.3 Hz, H-1'), 4.52 (m, 2H, H-2', H-3'), 4.42-4.20 (m, 5H, H-4', C*H*$_2$O-Tr, C*H*$_2$O-4), 3.90-3.70 (m, 2H, 5'C*H*$_2$) 3.90-3.23 (m, 8H, polyether C*H*$_2$).

**$O^4$-(3,6-Dioxa-8-hydroxy)octyluridine 5**

Compound **4** (250 mg, 0.40 mmole) was dissolved in 80% acetic acid and heated at 100°C for 10 min. Solvents were evaporated and the residue partitioned between water and ethyl ether, .Aqueous phase was extracted twice with ether and evaporated, leaving **5** as clear oil (128 mg, 034 mmole, 85 %). Elemental analysis ($C_{15}H_{24}N_2O_9$ ) calc. C 47.89%, H 6.43%, N 7.44%; found C 47.68%, H 6.66%, N 7.30%.

$^1$H NMR ($D_2O$) 8.18 (d, 2H, J=7.4 Hz, H-6), 6.25 (d, 1H. J=7.4 Hz, H-5), 5.90 (d, 1H, J=2.7 Hz, H-1'), 4.51-4.48 (m, 2H, H-2', H-3'), 4.35-4.11 (m, 5H, H-4', C*H*$_2$O-4, C*H*$_2$OH), 3.95-3.61 (m, 10 H, 5'C*H*$_2$, polyether C*H*$_2$).

$^{13}$C NMR ($CD_3OD$) 173.10 (C4), 158.19 (C2), 145.43 (C6), 97.03 (C5), 92.68 (C1'), 85.83 (C4'), 76.51, 73.69, 71.63, 71.33, 70.27, 69.99, 67.53, 62.22, 61.50 (C2', C3',C5', oxaethylene chain). Weak signals from N3-substituted isomer visible at 142.53, 102.66, 90.64, 86.83, 75.75, 62.30, 62.08.