Supplementary Information Presented with the Paper Entitled

Specific Recognition of Fluoride Anion Using a Metallamacrocycle Incorporating a Uranyl-Salen Unit.

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Warning: Care should be taken when handling uranyl containing compounds because of their toxicity and radioactivity.

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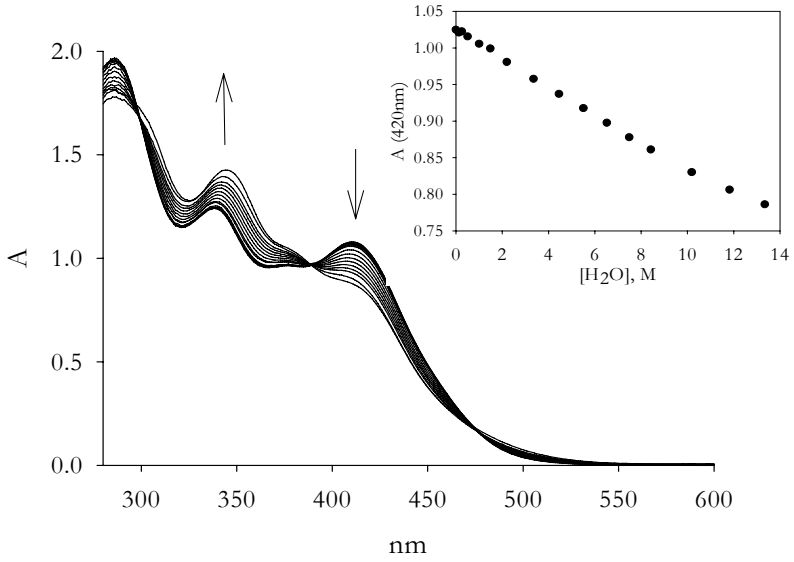


Figure S1: UV-Vis spectral changes of a 8.3×10^{-5} M 1:1 mixture of **1** and (TBA)F in DMSO upon addition of water. The inset shows spectral changes at λ=420 nm.

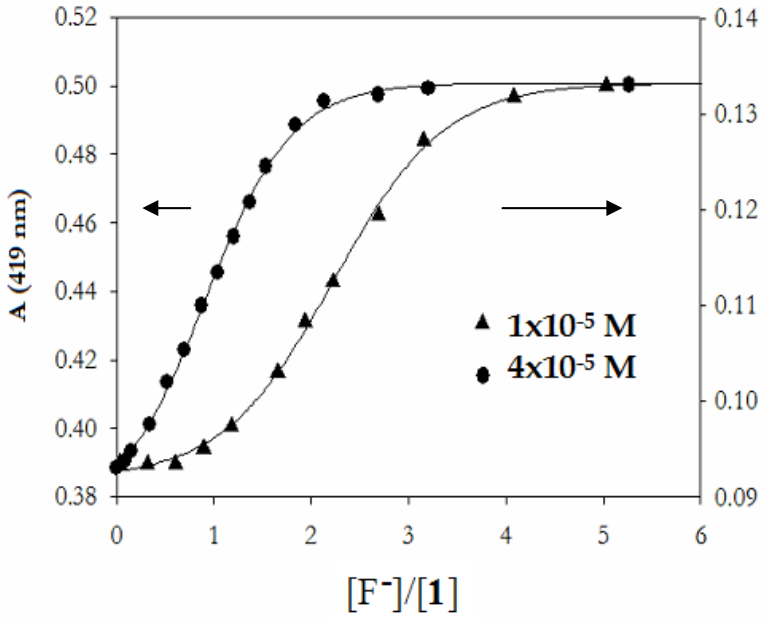


Figure S2: UV-Vis titration of receptor **1** with (TBA)F in DMSO at different concentrations.

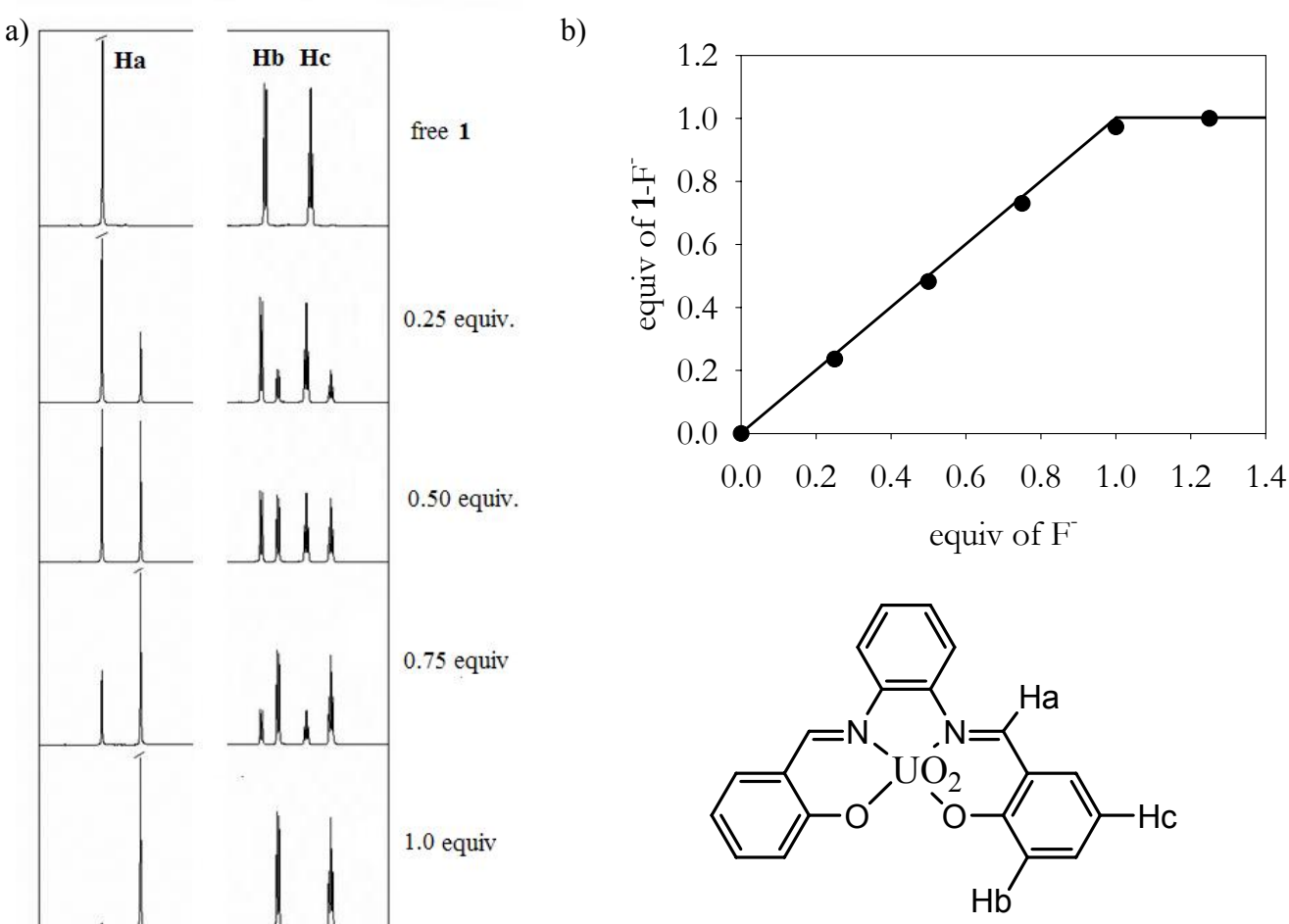
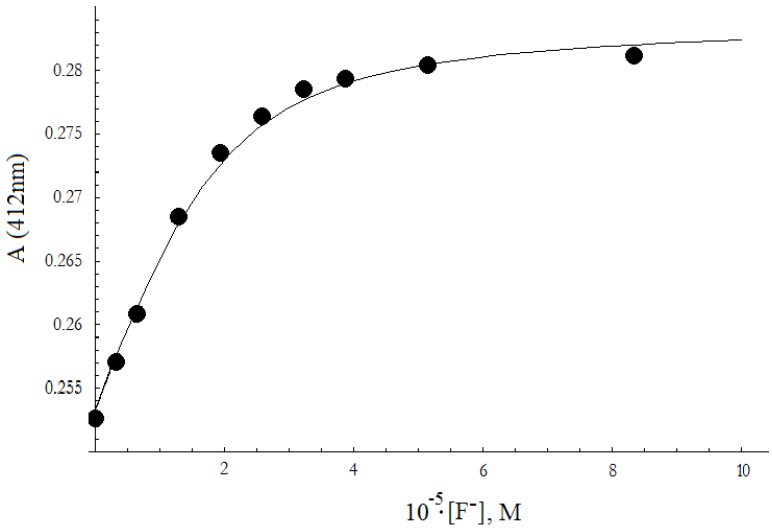


Figure S3: a) ^{1}H-NMR titration of a 1.2x10^{-3} M solution of **1** in DMSO-d_6 with (TBA)F. The portion of the spectra corresponding to the resonances of the proton *a*, *b* and *c* are shown. b)Titration profile for proton *a* which shows a 1:1 stoichiometry.

a)



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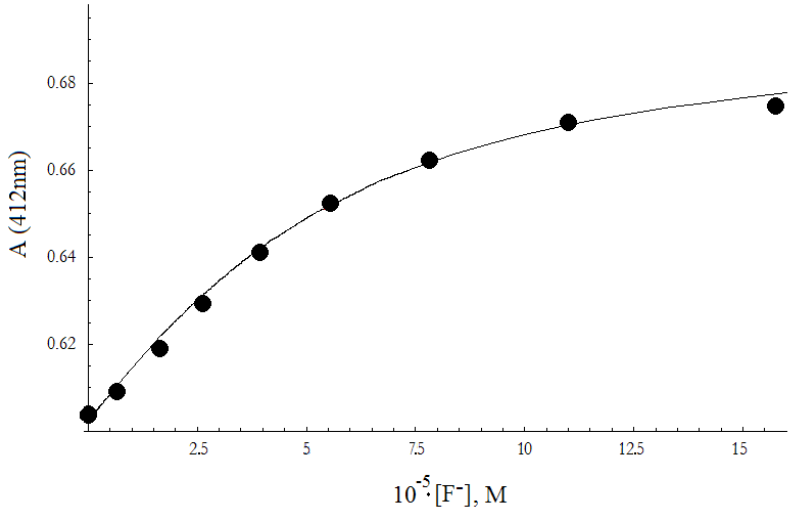


c)

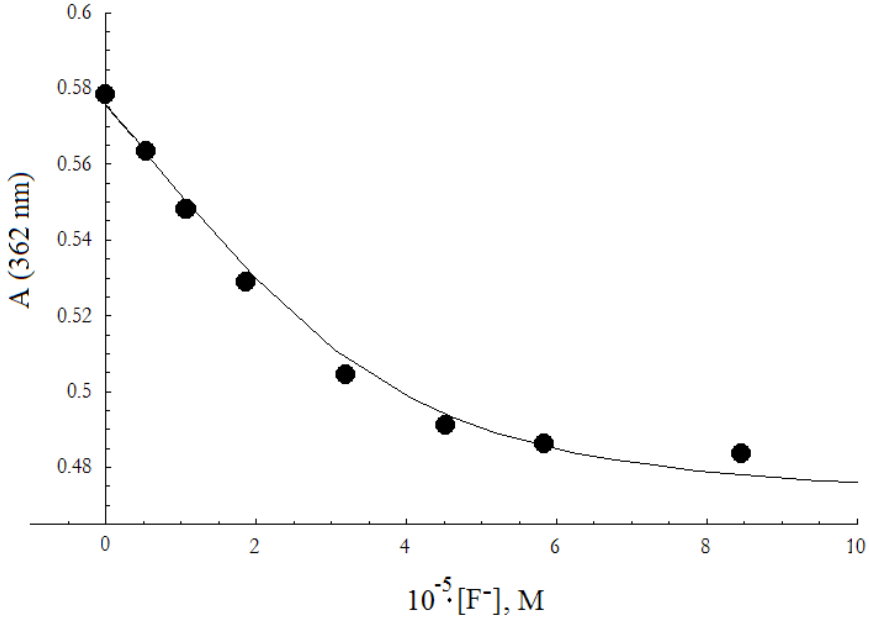


Figure S4: Competitive UV-Vis titration experiments with (TBA)F in the presence of excess (TMA)AcO. a) [**1**] = 2.0×10^{-5} M, [(TMA)AcO] = 2.0×10^{-3} M; b) [**1**] = 4.3×10^{-5} M, [(TMA)AcO] = 2.15×10^{-2} M; c) [**2**] = 4.7×10^{-5} M, [(TMA)AcO] = 2.35×10^{-2} M. Best fit of data points to eq 16 in ref 1 gave the following log K values: a) 6.5±0.15; b) 6.3±0.1; c) 6.5±0.2 The curves represent best fits to the above equation.

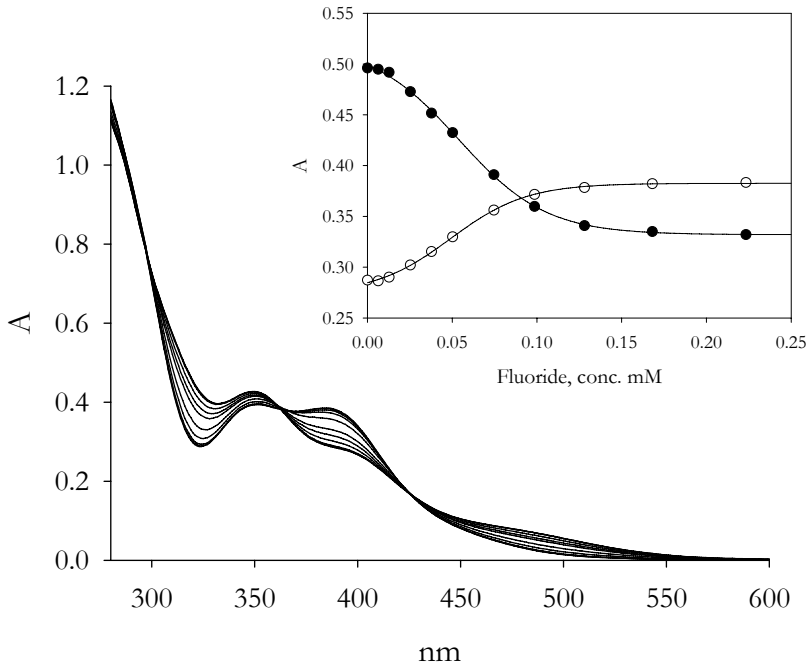


Figure S5: UV-Vis spectral changes of 4.87×10^{-5} M **3** upon addition of (TBA)F in DMSO, 25°C. The inset shows spectral changes at λ = 316 nm (●), and 388 nm (○).

X-ray Data Collection and Crystal Structure Determinations.

X-ray data for **3** were collected from orange needle-like crystal of size 0.05 x 0.3 x 0.5 mm on a Nonius Kappa CCD diffractometer using graphite monochromatized MoK_α radiation and the temperature of 173.0 K. Structure solution was performed by SHELXS-97 and refined on F^2 by full-matrix least-squares techniques (SHELXL-97).[2] Due to probable twinning of the crystal TWIN refinement was used. Hydrogen atoms were calculated to their idealised positions and refined as riding atoms (temperature factor 1.2 or 1.5 times C temperature factor). Absorption correction was applied in the final refinement.[3] One of the methanols in the crystal lattice was refined isotropically with site occupation factor of 0.5. Residual electron density over 1.00 $eÅ^{-3}$ was observed near uranium.

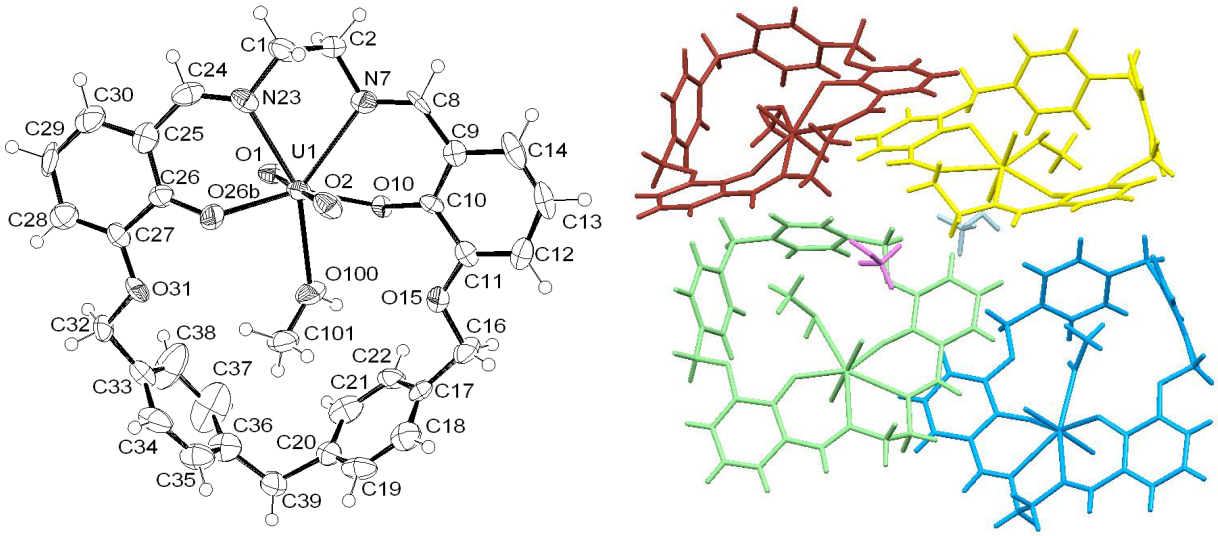
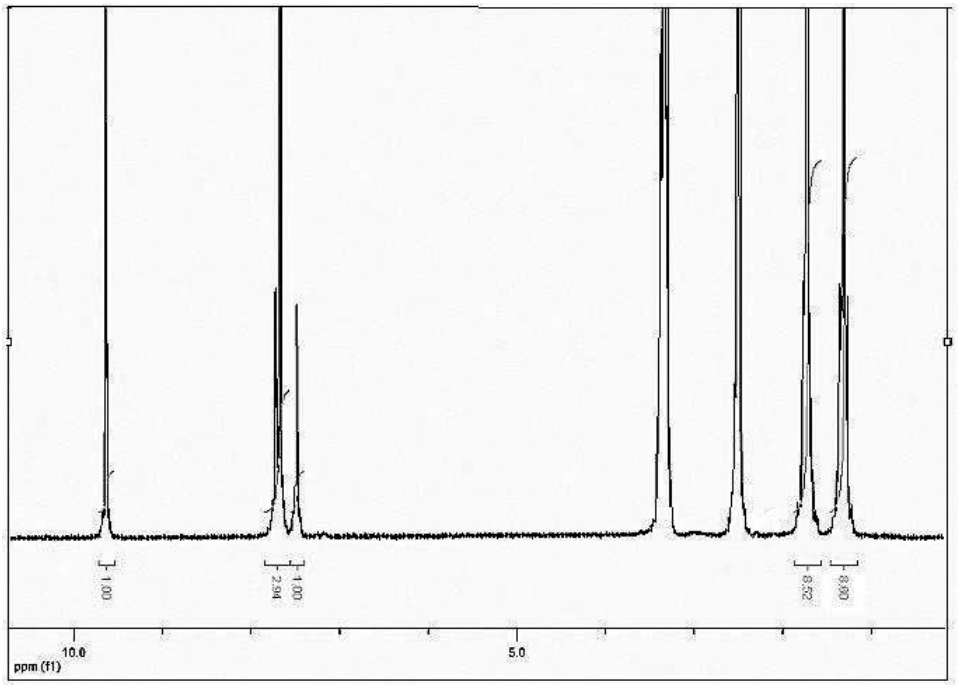


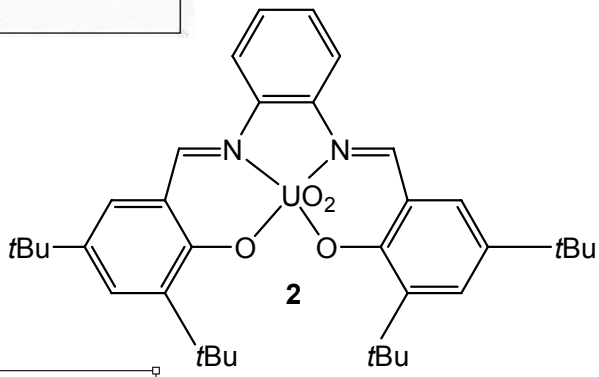
Figure S6: Complete crystallographic numbering of **3** (left) and the content of the asymmetric unit (right).

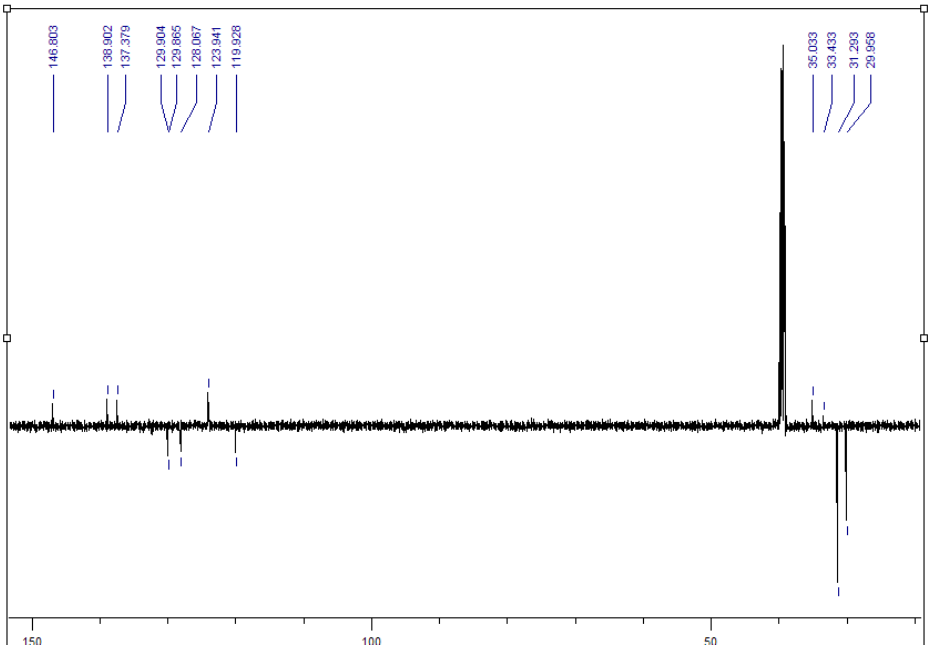
Receptor **2**:

^{1}H-NMR



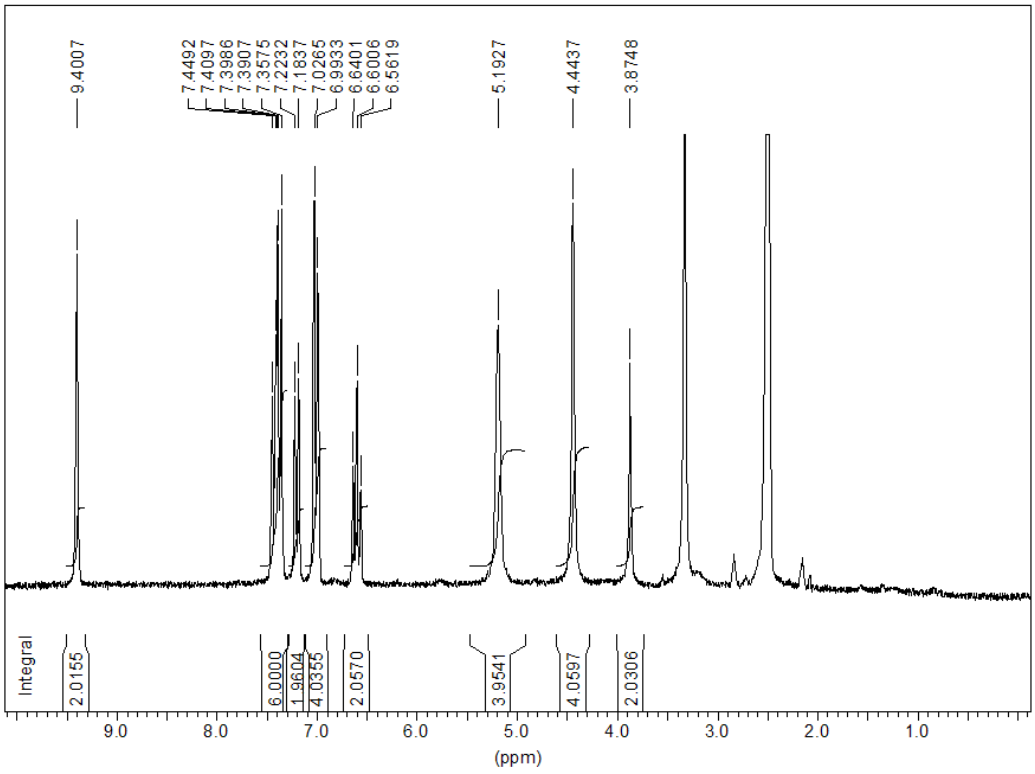
^{13}C NMR

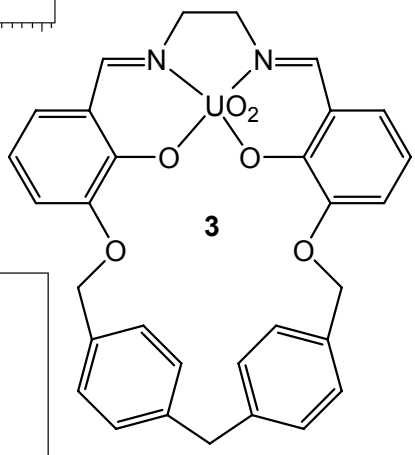




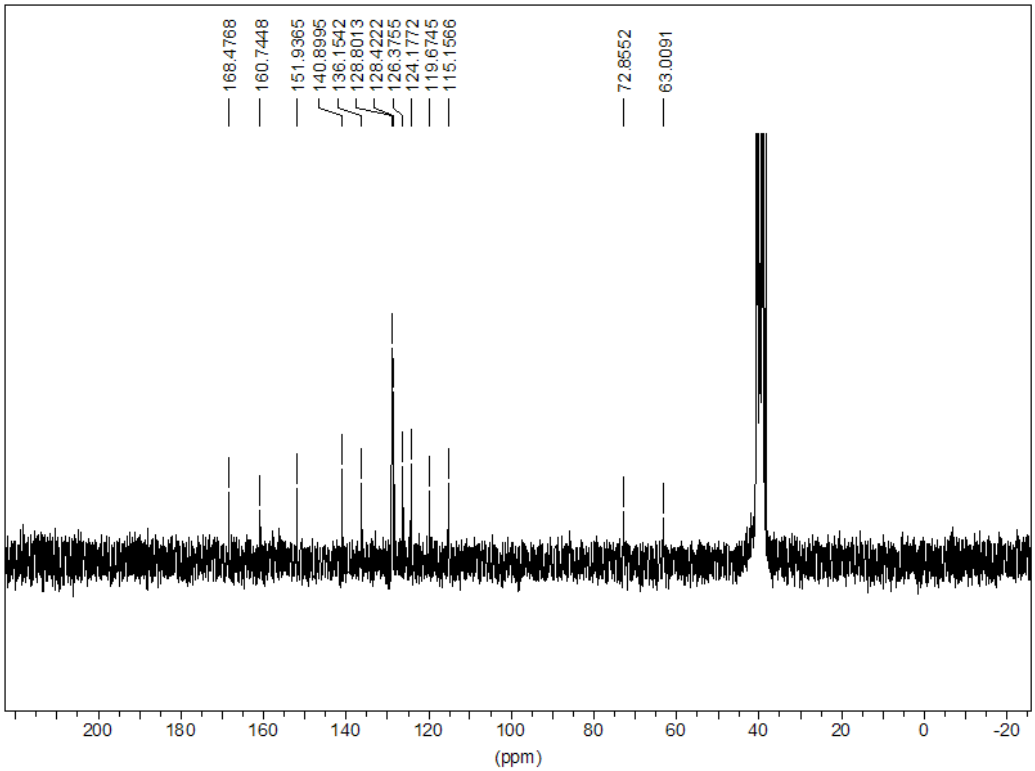
Receptor **3**

^{1}H NMR





^{13}C NMR



References

[1] Z.-X. Wang *FEBS Lett*., 1995, **360**, 111-114.

[2]SHELXS-97 and SHELXL-97: G. M. Sheldrick, *SHELX97 - Programs for Crystal Structure Analysis (Release 97-2).* Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

[3] R. H. Blessing, *Acta Crystallogr., Sect. A,* 1995, **51**, 33-38.