**Supplementary information**

# Macrocyclic receptor for pertechnetate and perrhenate anions

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## Contents

## General methods

All solvents were of reagent grade quality and purchased commercially. Starting materials were purchased from Aldrich Chemical Co., Acros Organics and used without further purification. NMR spectra used in the characterization of products were recorded on a Bruker Avance 600 spectrometer. The NMR spectra were referenced to solvent and the spectroscopic solvents were purchased from Cambridge Isotope Laboratories. All MALDI-TOF mass spectra were recorded on a Reflex 3 Bruker instrument. Elemental analyses were performed by INEOS Analytical Lab and are reported as percentages. TLC analyses were carried out using Baker-flex Silica gel IB-F sheets. Column chromatography was performed on Acros silica gel 60Å (230 – 400 mesh). 2,2´-(5-formyl-3-methyl-4-propyl-pyrrolyl)(p-tolyl)methane (**1**) was prepared according to the literature procedure.[1]

***Caution!*** Titrations were performed with $^{99}$Tc isotope, a low energy (0.292 MeV) $\beta^-$- particle emitter with a half-life of $2.12 \cdot 10^5$ years. When handled in milligram quantities ($[Tc]_0=10^{-3}$ □ $10^{-5}$M), $^{99}$Tc does not present a serious health hazard since common laboratory materials provide adequate shielding. Bremsstrahlung is not a significant problem due to the low energy of the $\beta^-$-particle emission. Normal radiation safety precautions were followed at all times to prevent contamination.

**Abbreviations:**

TEA – triethylamine

DMAP – 4-dimethylaminopyridine

DCM – dichloromethane

DHB – 2,4-dihydroxybenzoic acid

DCE – 1,2-dichloroethane

DMSO – dimethylsulfoxide

## Spectra of receptors

**Bis(3-aminophenyl)pyridine-2,6-dicarboxamide (2).**

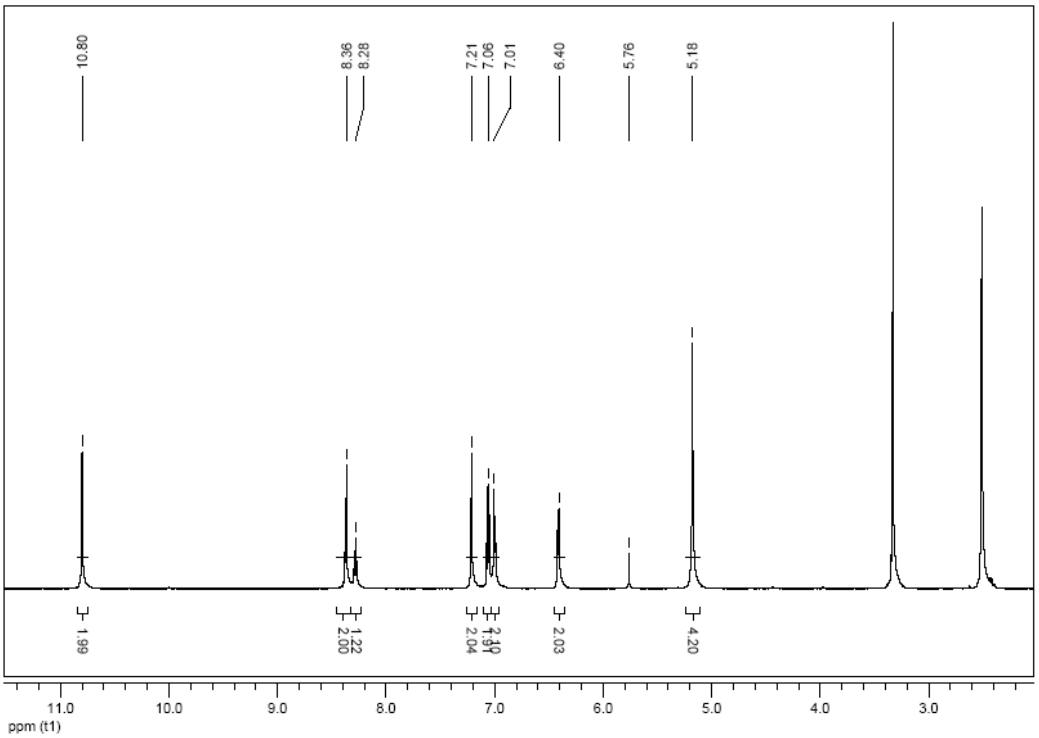



**Figure S1.** $^{1}$H NMR of **2**

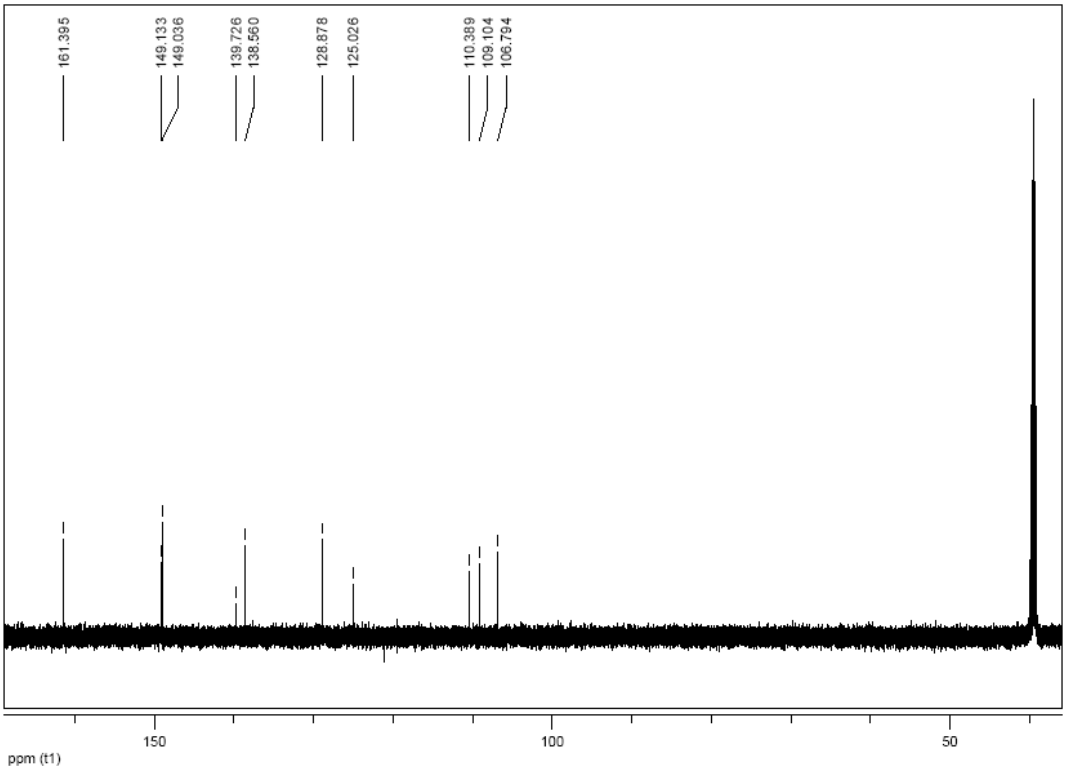
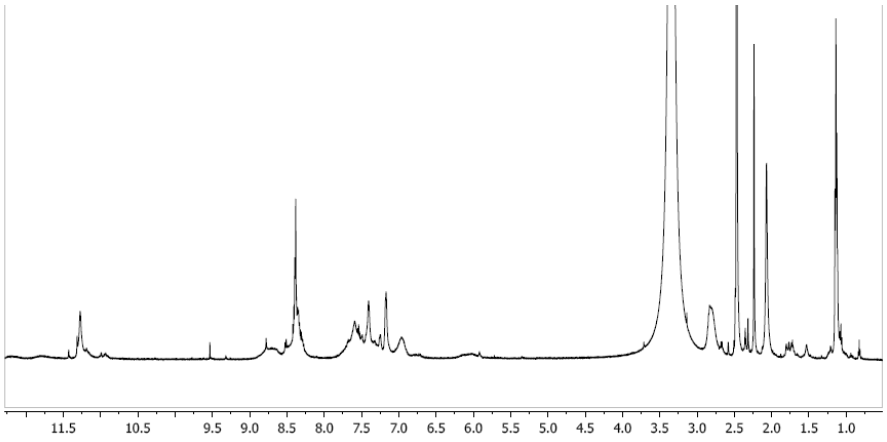



**Figure S2.** $^{13}$C NMR of **2**

**General procedure for synthesis of macrocycle *L*[1].**

Diamine **2** 43.0 mg (0.12 mmol) and dialdehyde **1** 50.0 mg (0.12 mmol) were dissolved in 1 ml of methanol and stirred for 10 minutes. Then 2.5 eq. of template acid was added to a solution ($HCl_{conc}$ (26%), $H_2SO_4$ $_{conc}$ (98%), $HClO_4$ $_{conc}$ (70%) or $HReO_4$ $_{conc}$ (70%)). The mixture was allowed to react for the next 10 hours under r.t. The red colored precipitate formed was filtered off yielding the macrocyclic product as a salt of corresponding acid. The solid was dissolved in 95:5 (v/v) DCM-MeOH solution and layered with hexane. The resulting crystals were dissolved in 95:5 (v/v) DCM-MeOH and treated with 3.3 ml (2.4 mmol) of triethylamine and evaporated. The product was passed through alumina plug (eluent 95:5 (v/v) DCM-MeOH) yielding free base as a yellow-red powder.

**Macrocycle *L*[1] (R=Pr).**



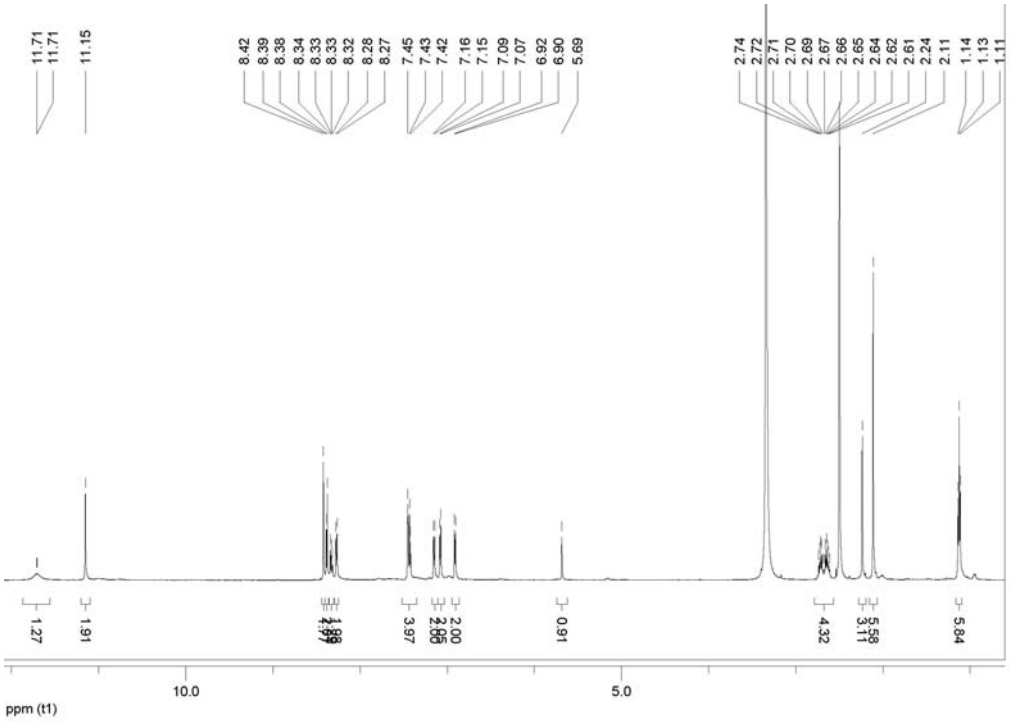



**Figure S3.** $^{1}$H NMR of the crystals of $\boldsymbol{L^1}$•2HReO$_4$ in DMSO D$_6$ and free $\boldsymbol{L^1}$ which is obtained by neutralization of the former with the help of triethylamine.

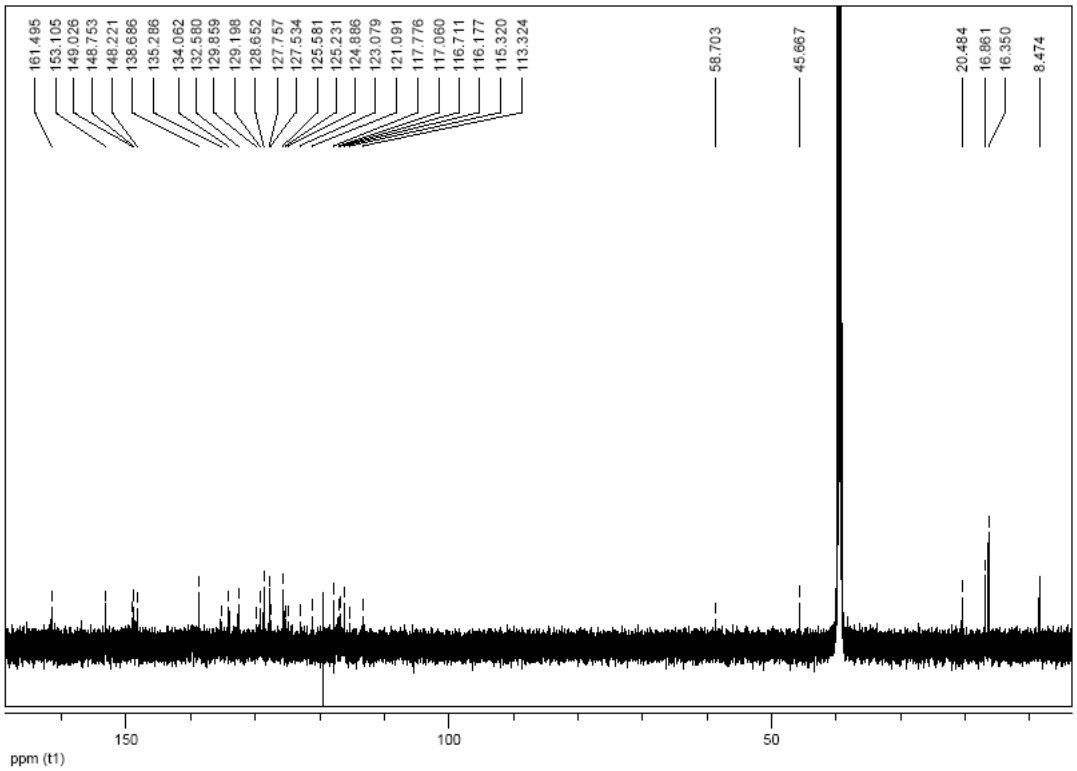



**Figure S4.** $^{13}$C NMR of $\boldsymbol{L^1}$.

**5,5'-(propane-2,2-diyl)bis(N-(3-aminophenyl)-4-methyl-3-phenyl-1H-pyrrole-2-carboxamide) (3).**

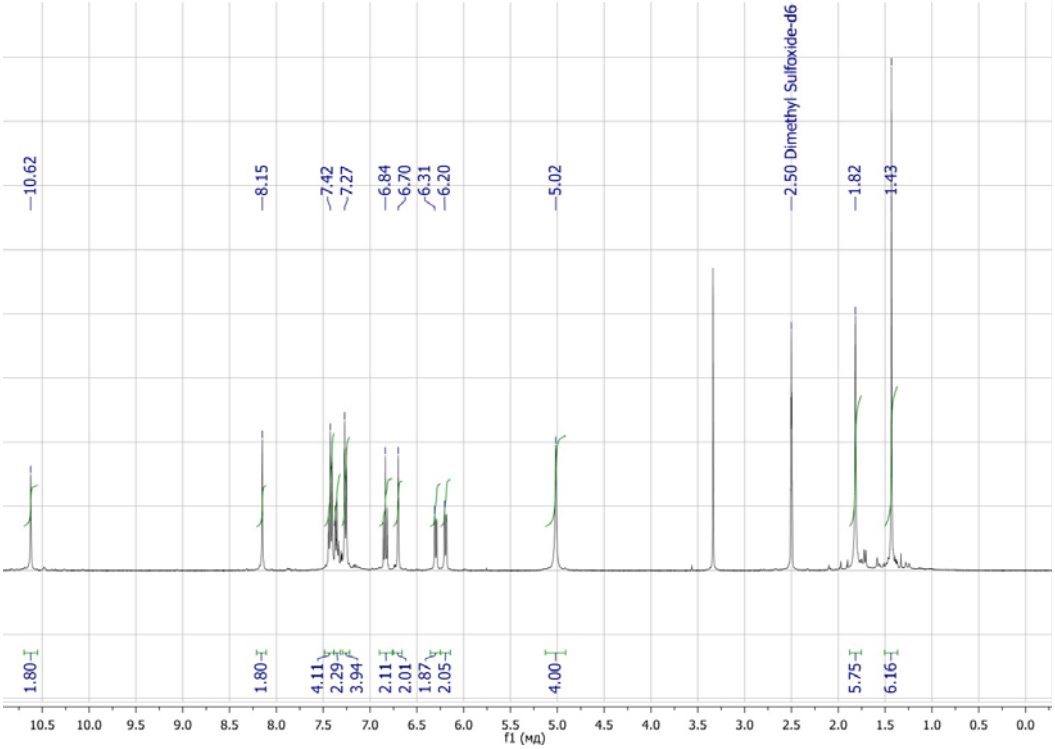



**Figure S5.** $^{1}$H NMR of **3**

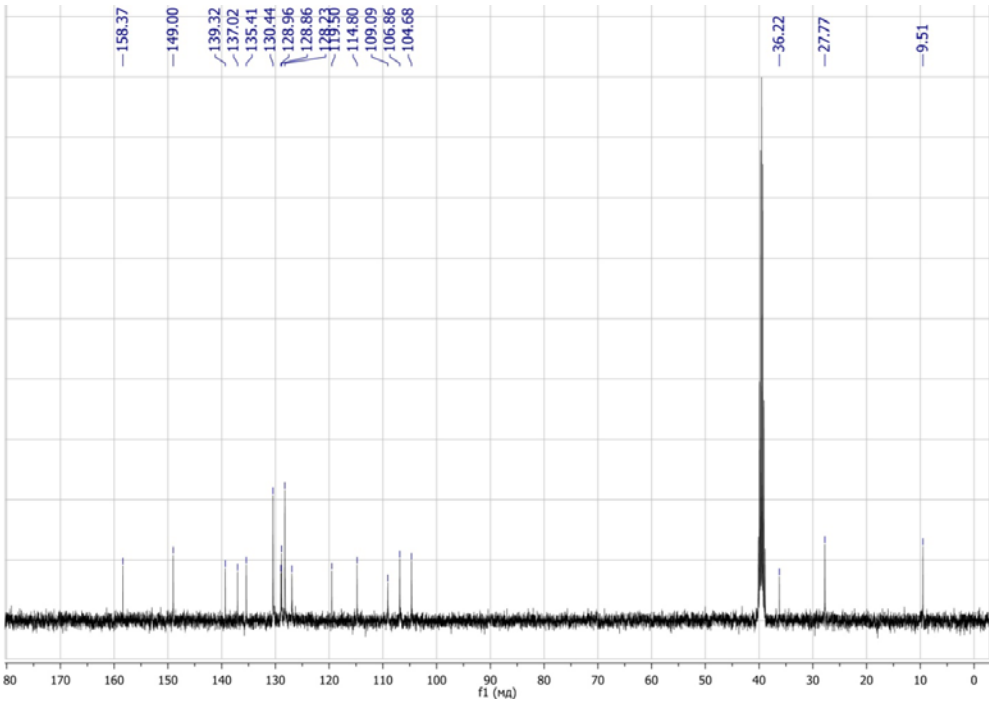



**Figure S6.** $^{13}$C NMR of **3**

**Macrocycle *L*$^2$**

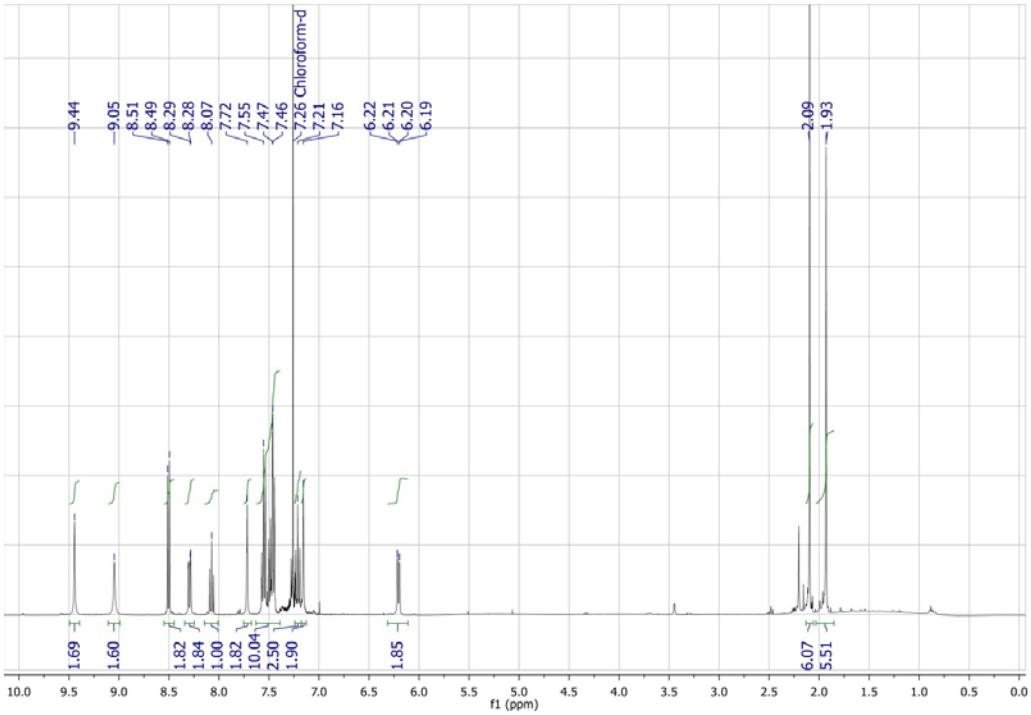



**Figure S7.** $^1$H NMR of ***L*$^2$**

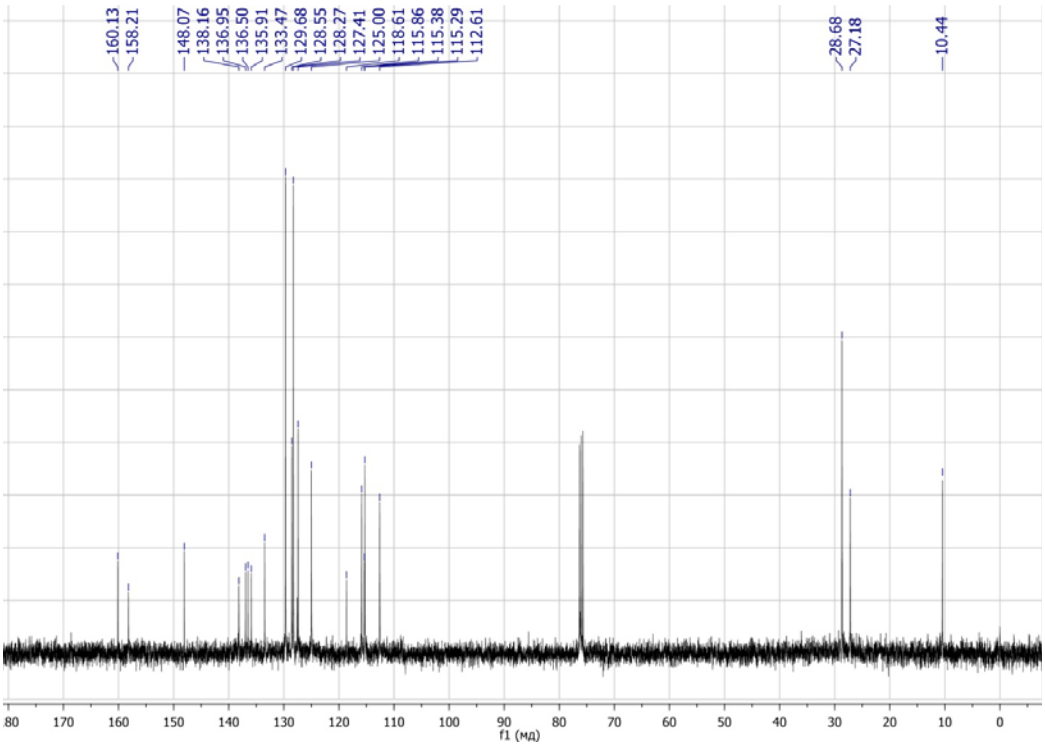



**Figure S8.** $^{13}$C NMR of ***L*$^2$**

## Job Plot Construction

A stock solution of the host was prepared as described for the $K_a$ determination experiments. The guest stock solution was prepared by dissolving 1 - 2 equivalents of the tetrabutylammonium salts of the studied anions is the same solvent (acetonitrile) as the one used for the host stock solution.

The general procedure for the UV-Vis Job titrations involved making sequential additions of titrant (anionic guest) using Hamilton® pipettes to a 1.5 ml aliquot of the host stock solution in a spectrometric cell. The data was then collated and combined to produce data files from which so-called Job plots could be constructed. These latter were produced as described by Connors, namely by plotting the molar fraction of guest ($X_G$) as a function of [host] × ΔA. The plots themselves were generated using Origin version 7.5. The change in absorbance, ΔA, was calculated at a λ value where the spectral change was maximal. Maximum of the resulting graph was considered indicative of the stoichiometry of the host:guest complex, namely a maximum $X_G = 0.5$ is considered indicative of a 1:1 host:guest complex, while $X_G = 0.33$ is considered 2:1 host:guest stoichiometry.

## $^{99}$Tc NMR titration

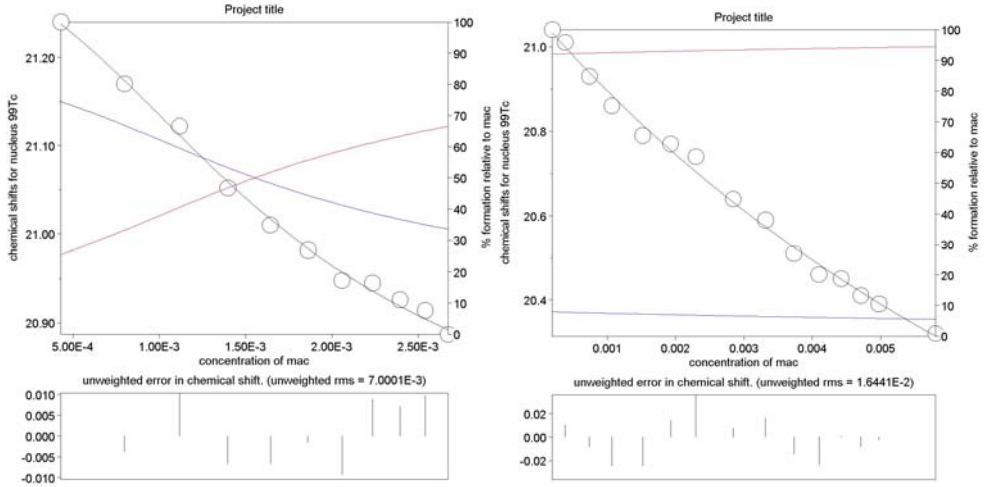



**Figure S9.** Fitting curves of reverse $^{99}$Tc NMR titrations for receptors $\mathbf{L^1}$ (left) and $\mathbf{L^2}$ (right). The curves are exported from HYPERNMR2006 program. Rounds □ experimental points, black line □ fitting curve, blue line □ concentration of TBA$^{99}$TcO4, red line □ concentration of host-guest complex.

## X-ray structure determination

### Complex $L^1$•2$HReO_4$

Data were collected on a Bruker SMART APEX II CCD diffractometer ($\lambda$(Mo$K_\alpha$)-radiation, graphite monochromator, $\omega$ and $\varphi$ scan mode) and corrected for absorption using the *SADABS* program.[2] For details, see **Table S1**. The structure was solved by direct methods and refined by a full-matrix least squares technique on $F^2$ with anisotropic displacement parameters for non-hydrogen atoms. The independent part of the unit cell of **$L^1$•2($HReO_4$)** contains two 1,2-dichloroethane solvate molecules. One of the two solvate molecules occupies a special position on the inversion center with the total positional occupancy of 0.5, and the other molecule has total positional occupancy of 0.25. The hydrogen atoms were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters ($U_{iso}$(H) = 1.5$U_{eq}$(C) for the $CH_3$-groups and $U_{iso}$(H) = 1.2$U_{eq}$(N or C) for the other groups). All calculations were carried out using the *SHELXTL* program.[3] Crystallographic data for **$L^1$•2 $HReO_4$**·½($C_2H_4Cl_2$) have been deposited with the Cambridge Crystallographic Data Center. **CCDC 696738** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

**Table S1**. Crystal data and structure refinement for **$L^1$•2($HReO_4$)**•½($C_2H_4Cl_2$)

| | | |
|---|---|---|
| Empirical formula | C46 H49 Cl N7 O10 Re2 | |
| Formula weight | 1267.77 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 11.247(6) Å | α = 94.835(9)°. |
| | b = 15.201(8) Å | β = 97.922(10)°. |
| | c = 15.814(8) Å | γ = 102.318(9)°. |
| Volume | 2598(2) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.621 $Mg/m^3$ | |
| Absorption coefficient | 4.765 $mm^{-1}$ | |

| | |
|---|---|
| F(000) | 1242 |
| Crystal size | 0.15 x 0.12 x 0.03 $mm^3$ |
| Theta range for data collection | 3.09 to 25.00°. |
| Index ranges | -13<=h<=13, -18<=k<=18, -18<=l<=18 |
| Reflections collected | 22216 |
| Independent reflections | 9053 [R(int) = 0.0834] |
| Completeness to theta = 25.00° | 98.9 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.870 and 0.535 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 9053 / 93 / 318 |
| Goodness-of-fit on $F^2$ | 0.920 |
| Final R indices [for 2186 rflns with I>2σ(I)] | R1 = 0.0755, wR2 = 0.1024 |
| R indices (all data) | R1 = 0.2442, wR2 = 0.1561 |
| Largest diff. peak and hole | 1.025 and -1.031 $e.Å^{-3}$ |

**Table S2**. Hydrogen bonds for **$L^1$•2($HReO_4$)** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N1-H1A...O1 | 0.86 | 2.38 | 3.129(17) | 146 |
| N2-H2A...O1 | 0.86 | 2.16 | 2.927(17) | 148 |
| N2-H2A...O5 | 0.86 | 2.43 | 2.911(17) | 116 |
| N3-H3A...O4 | 0.86 | 2.75 | 3.363(16) | 130 |
| N5-H5A...O4 | 0.86 | 2.88 | 3.445(16) | 125 |
| N6-H6A...O6 | 0.86 | 1.94 | 2.758(17) | 159 |
| N7-H7A...O6 | 0.86 | 2.12 | 2.926(18) | 156 |
| C7-H7B...O7 | 0.93 | 2.88 | 3.561(15) | 142 |
| C20-H20A...O7 | 0.93 | 2.38 | 3.201(15) | 147 |

**Complex $L^1$•2HCl**

Data were collected on a Bruker SMART APEX II CCD diffractometer ($\lambda$(MoK$_\alpha$)-radiation, graphite monochromator, $\omega$ and $\varphi$ scan mode) and corrected for absorption using the *SADABS* program.[2] For details, see **Table S3**. The structure was solved by direct methods and refined by a full-matrix least squares technique on $F^2$ with anisotropic displacement parameters for non-hydrogen atoms. One of the two chloride anions is disordered over two sites with the occupancies of 0.6:0.4. The independent part of the unit cell of **$L^1$•2(HCl)** contains a dichloromethane solvate molecule. The hydrogen atoms were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters ($U_{iso}$(H) = 1.5$U_{eq}$(C) for the $CH_3$-groups and $U_{iso}$(H) = 1.2$U_{eq}$(N or C) for the other groups). All calculations were carried out using the *SHELXTL* program.[3] Crystallographic data for **$L^1$•2HCl** $C_2H_4Cl_2$ have been deposited with the Cambridge Crystallographic Data Center. **CCDC 818214** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

**Table S3**. Crystal data and structure refinement for **$L^1$•2HCl**•$C_2H_4Cl_2$.

| | | |
|---|---|---|
| Empirical formula | C44 H45 Cl4 N7 O2 | |
| Formula weight | 845.67 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1/c$ | |
| Unit cell dimensions | a = 16.89(4) Å | α = 90°. |
| | b = 15.29(4) Å | β = 110.63(3)°. |
| | c = 16.64(4) Å | γ = 90°. |
| Volume | 4023(16) Å$^3$ | |
| Z | 4 | |
| Density (calculated) | 1.396 Mg/m$^3$ | |
| Absorption coefficient | 0.343 mm$^{-1}$ | |
| F(000) | 1768 | |
| Crystal size | 0.15 x 0.12 x 0.08 mm$^3$ | |
| Theta range for data collection | 2.47 to 25.00°. | |
| Index ranges | -20<=h<=20, -18<=k<=18, -19<=l<=19 | |

| | |
|---|---|
| Reflections collected | 33694 |
| Independent reflections | 7016 [R(int) = 0.1104] |
| Completeness to theta = 25.00° | 99.1 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.973 and 0.950 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7016 / 0 / 528 |
| Goodness-of-fit on $F^2$ | 0.876 |
| Final R indices [for 1635 rflns with $I>2\sigma(I)$] | R1 = 0.0906, wR2 = 0.1391 |
| R indices (all data) | R1 = 0.3707, wR2 = 0.2213 |
| Largest diff. peak and hole | 0.534 and -0.399 e.$Å^{-3}$ |

**Table S4**. Hydrogen bonds for **$L^1$•2HCl** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N1-H1N...Cl1 | 0.88 | 2.27 | 3.140(8) | 169 |
| N2-H2N...Cl1 | 0.88 | 2.27 | 3.142(8) | 171 |
| N6-H6N...Cl1 | 0.88 | 2.30 | 3.138(8) | 159 |
| N7-H7N...Cl1 | 0.88 | 2.29 | 3.114(8) | 156 |
| C7-H7...Cl1 | 0.96 | 2.82 | 3.609(9) | 140 |
| C20-H20...Cl1 | 0.96 | 2.80 | 3.622(9) | 144 |
| N3-H3N...Cl2’ | 0.88 | 2.15 | 2.979(8) | 157 |
| N5-H5N...Cl2’ | 0.88 | 2.29 | 3.139(8) | 162 |
| C7-H7...Cl2’ | 0.96 | 2.80 | 3.417(9) | 123 |
| C20-H20...Cl2’ | 0.96 | 2.73 | 3.487(9) | 137 |

## Combinatorial experiments for macrocycle L[1] formation.

**Table S5**. Products of [n+n]-condensation generated using different templating acids.

| Reaction | HA | [1+1] | [2+2] | [3+3] | [4+4] |
|---|---|---|---|---|---|
| **1(R=Et) +2** | $H_3PO_4$ | + | + | – | – |
| | $H_2SO_4$ | + | + | – | – |
| | HCl | + | – | – | – |
| | $HReO_4$ | + | – | – | – |
| | $HClO_4$ | + | – | – | – |
| | $HNO^3$ | + and unknown byproduct | - | - | - |
| | no template | + low yield | | | |

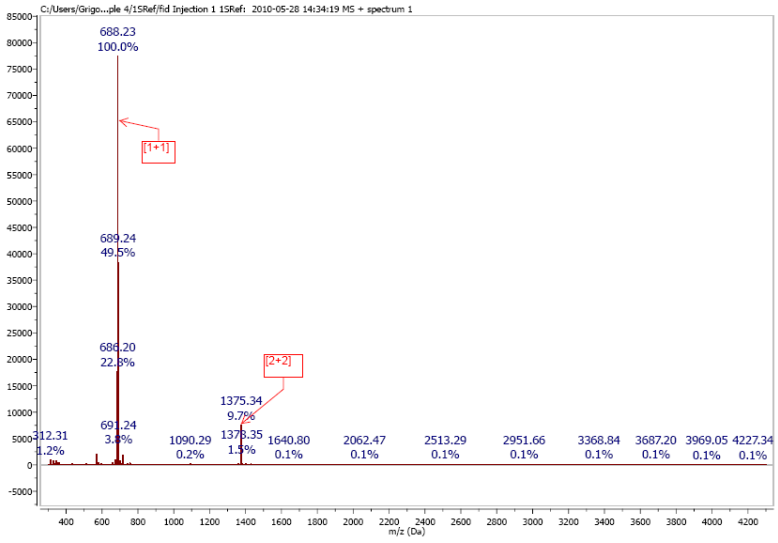



**Figure S10.** MALDI-TOF spectrum of the precipitate formed with $H_3PO_4$.

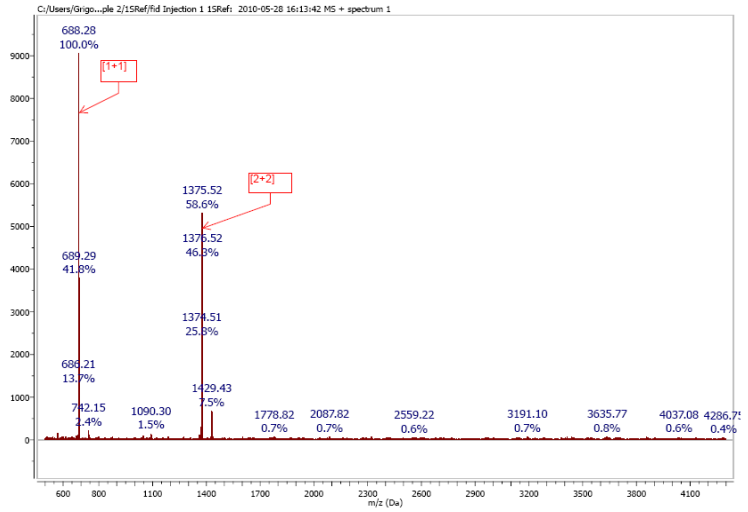



**Figure S11.** MALDI-TOF spectra of the precipitate formed with $H_2SO_4$.

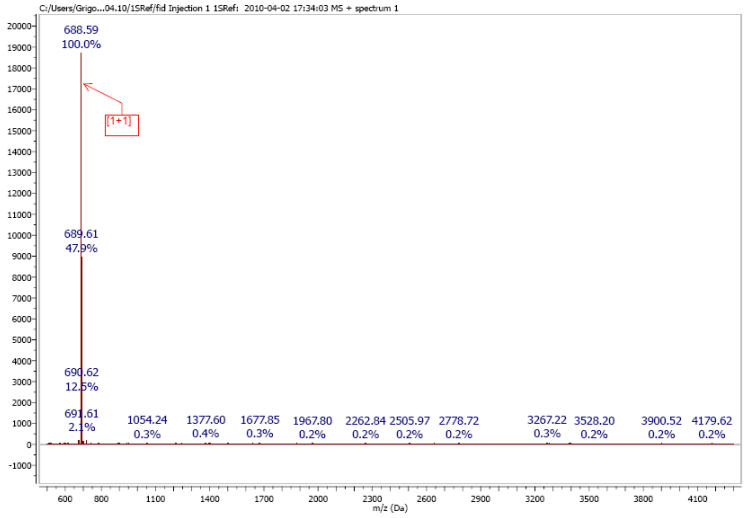



**Figure S12.** MALDI-TOF spectrum of the precipitate formed with HCl.

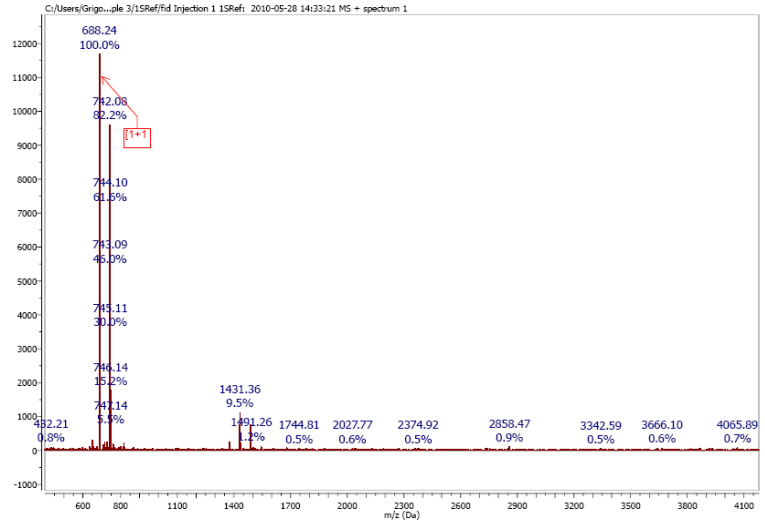



**Figure S13.** MALDI-TOF spectrum of the precipitate formed with $HNO_3$.

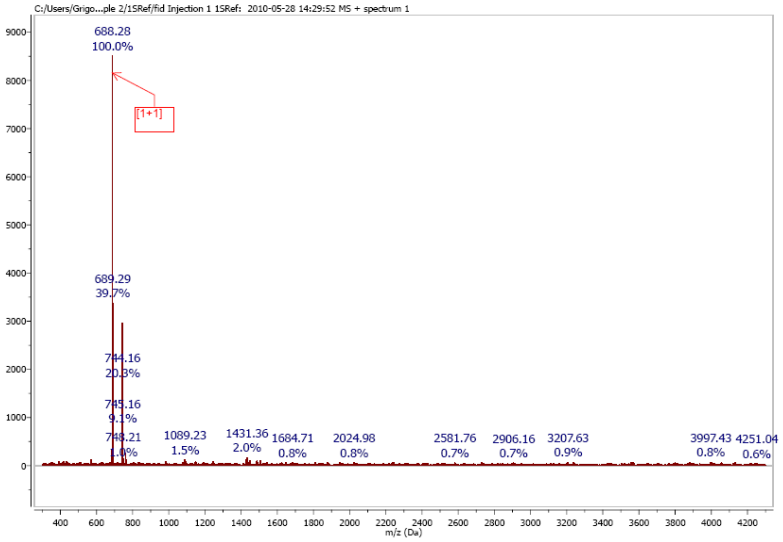



**Figure S14.** MALDI-TOF spectrum of the precipitate formed with $HClO_4$.

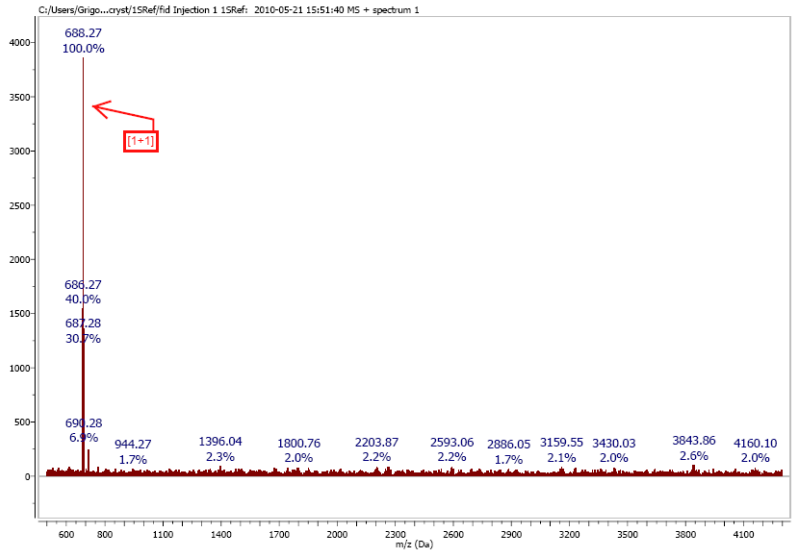


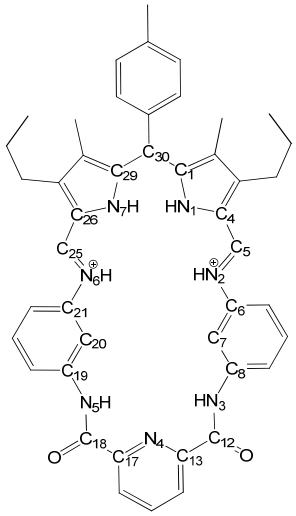

**Figure S15.** MALDI-TOF spectrum of the precipitate formed with $HReO_4$.

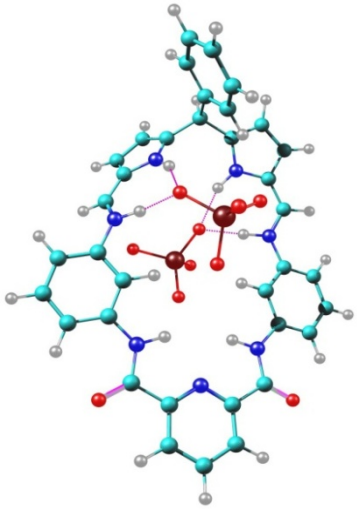
## DFT calculations

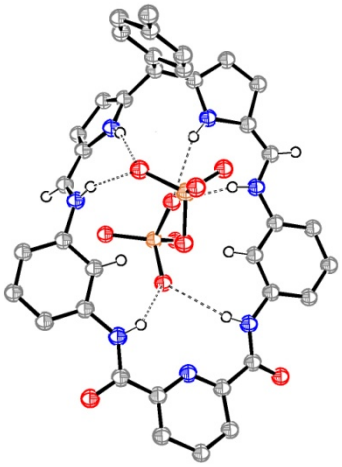
Molecular modeling calculations were performed using the DFT program "PRIRODA 2006".[4] A PBE function that includes the electron density gradient was used. The TZ2p-atomic basis sets of grouped Gaussian functions were used to solve the Kohn-Sham equations. The criterion for convergence was a difference below 0.01 kcal/mol/Angstrom in energy between two sequential structures. Various stationary points on the potential energy surface (PES) were determined from analytical calculations of the second energy derivatives (Hessian matrixes).

**Table S6**. Comparison of structural parameters of the optimized structure and the structure obtained from the X-ray analysis.

| $\mathbf{L^1 \cdot 2}HReO_4$ | | |
|---|---|---|
| Structure | Theoretically predicted structure | Structure according to the X-ray analysis |



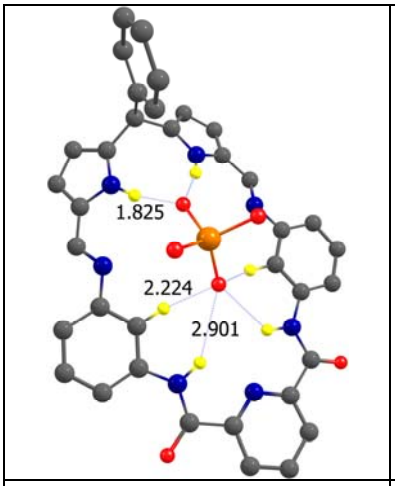



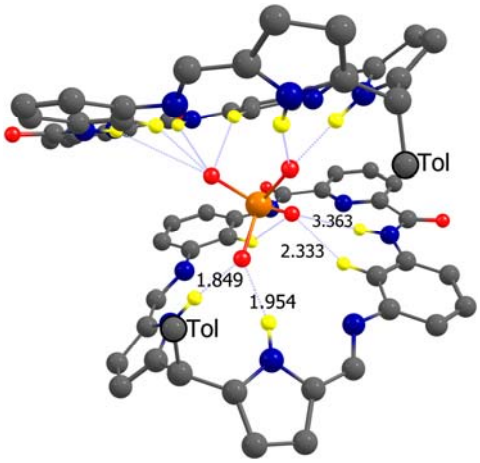


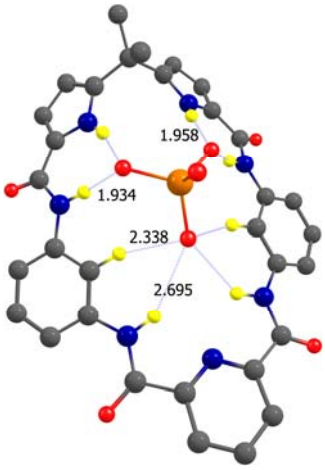
| Тип и характер расстояния | | $L_{theor}$, Å | $L_{X\text{-}ray}$, Å | $\lvert L_{theor} - L_{X\text{-}ray} \rvert$, Å |
|---|---|---|---|---|
| Размер **49** | **C30 – N4** | 10.60 | 10.34 | 0.26 |
| | **C7 – C20** | 5.63 | 5.65 | 0.02 |
| | **C5 – C25** | 7.04 | 7.16 | 0.12 |
| | **N2 – N6** | 6.25 | 6.33 | 0.08 |
| | **N3 – N5** | 4.60 | 4.66 | 0.06 |
| **Re1**$O_4$ – **Re2**$O_4$ | **Re1 – Re2** | 5.00 | 4.90 | 0.10 |
| | **O5 – O1** | 2.71 | 2.76 | 0.04 |
| | **O6 – O3** | 2.78 | 2.93 | 0.15 |
| | **O7 – O4** | 3.25 | 3.25 | 0.00 |
| **Re1**$O_4$ – **49** | **O3 – N6** | 4.12 | 4.14 | 0.01 |
| | **O3 – N7** | 3.72 | 3.60 | 0.12 |
| | **O1 – N1** | 4.93 | 4.99 | 0.06 |
| | **O1 – N2** | 3.48 | 3.38 | 0.09 |
| | **O4 – N4** | 3.24 | 3.16 | 0.08 |
| **Re2**$O_4$ – **49** | **O6 – N6** | 3.11 | 2.91 | 0.20 |
| | **O6 – N7** | 2.82 | 3.13 | 0.31 |
| | **O5 – N1** | 2.76 | 2.93 | 0.17 |
| | **O5 – N2** | 4.20 | 3.64 | 0.56 |
| | **O7 – N4** | 4.50 | 4.55 | 0.05 |

| | | |
|---|---|---|
| Pirson coefficient | 0.995 | Error range: |
| Correlation coefficient | 0.995 | 0.13 ± 0.06 Å (95% probability) |
| $\chi^2$-test | 1.000 | 0.13 ± 0.08 Å (99% probability) |

**Table S7**. Views and Cartesian coordinates of the optimized structures $\mathbf{L^1}$•$ReO_4^-$. 2$\mathbf{L^1}$•$ReO_4^-$, $\mathbf{L^2}$•$ReO_4^-$.

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| 1 | -7.895232260 | 0.391321830 | -5.314609470 |
| 1 | -6.208761530 | 2.380574180 | -4.447347810 |
| 1 | -2.786116590 | -5.071856860 | -4.828962120 |
| 1 | -5.742587230 | -2.835102410 | -2.626343300 |
| 1 | -5.032068400 | -3.952080000 | -0.531886770 |
| 1 | -3.191378330 | -5.640675490 | -0.571023980 |
| 1 | -2.073586870 | -6.194208240 | -2.732928780 |

| | | | |
|---|---|---|---|
| 1 | 3.133640200 | -5.049413010 | -3.244810450 |
| 6 | 3.767195230 | -3.269812270 | 0.669959100 |
| 1 | 5.522995610 | -2.262002800 | -3.178108060 |
| 1 | 3.143580230 | -0.699959240 | -0.047305380 |
| 1 | 5.424867480 | 0.452374500 | -3.414567640 |
| 8 | 4.235228390 | 2.635929420 | -2.176704220 |
| 1 | -0.836214690 | -2.639632100 | -0.019276210 |
| 1 | 5.954042710 | -3.930938030 | -0.817464590 |
| 1 | 4.788515360 | -5.287651940 | -0.852360620 |
| 1 | 5.136771590 | -4.369270620 | -2.333156750 |
| 1 | 4.717672240 | -2.919513030 | 1.097582720 |
| 1 | 2.977089020 | -2.600879840 | 1.036593900 |
| 1 | 3.554126190 | -4.274466030 | 1.062685870 |
| 75 | 0.705759010 | -0.677861830 | 2.264375620 |
| 8 | 0.949704890 | -0.935102340 | 3.960466230 |
| 8 | 0.321857850 | -2.201283700 | 1.464957120 |
| 8 | -0.602575430 | 0.455715670 | 2.003238750 |
| 8 | 2.176511270 | -0.047254670 | 1.525165680 |

## NMR kinetics measurements of macrocyclization

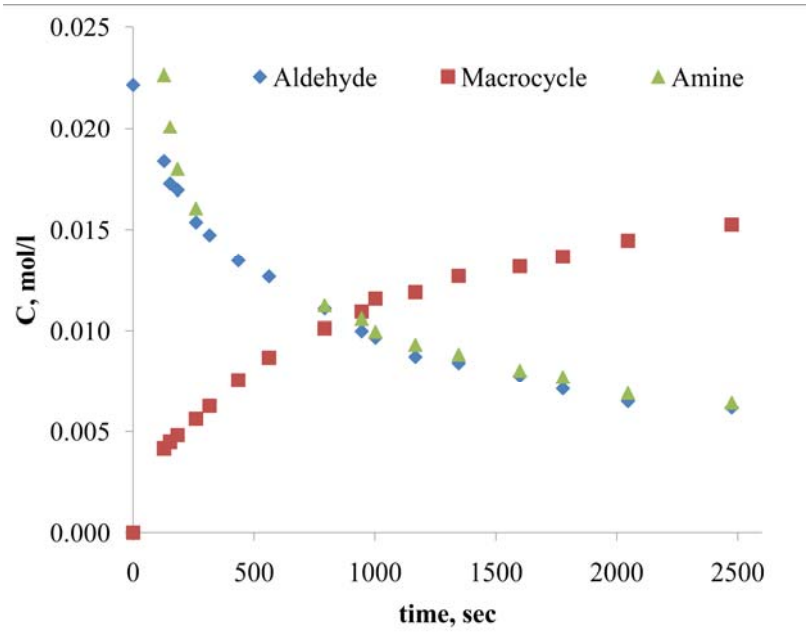
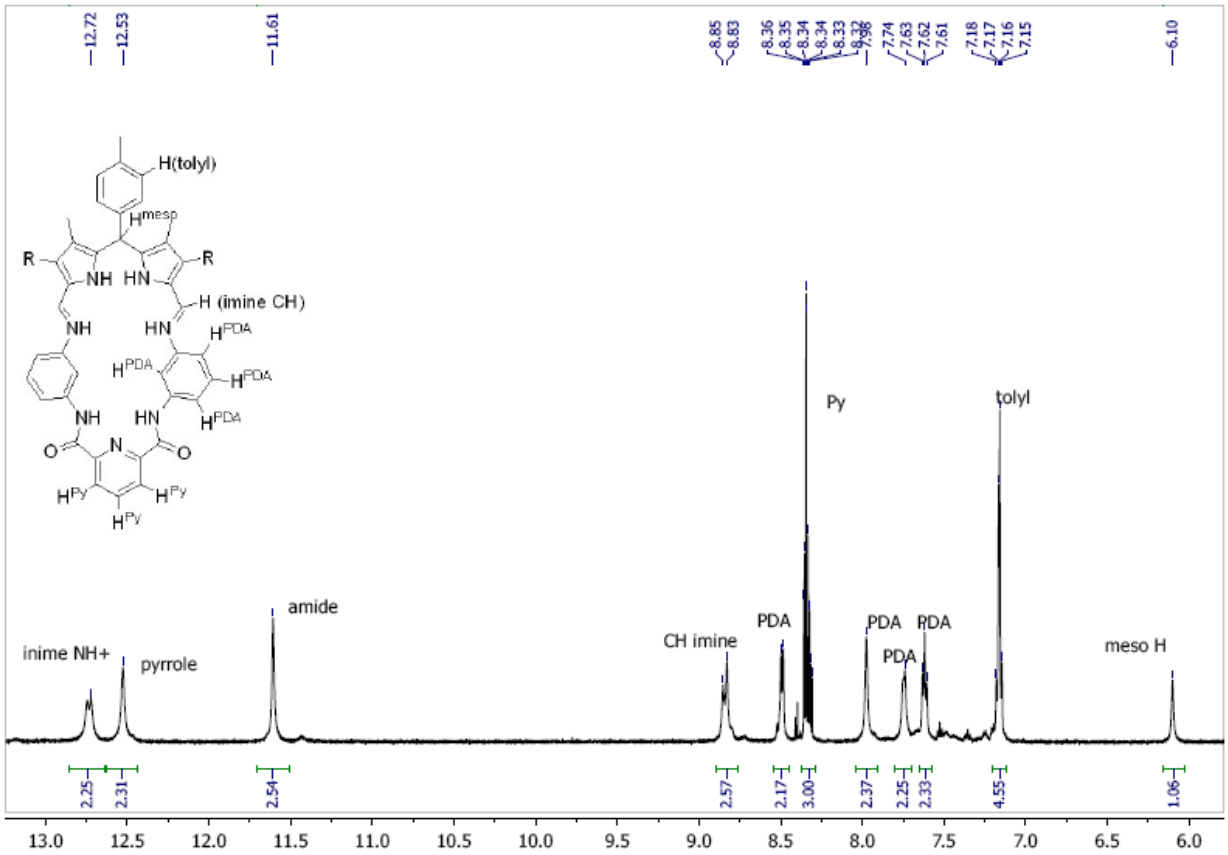
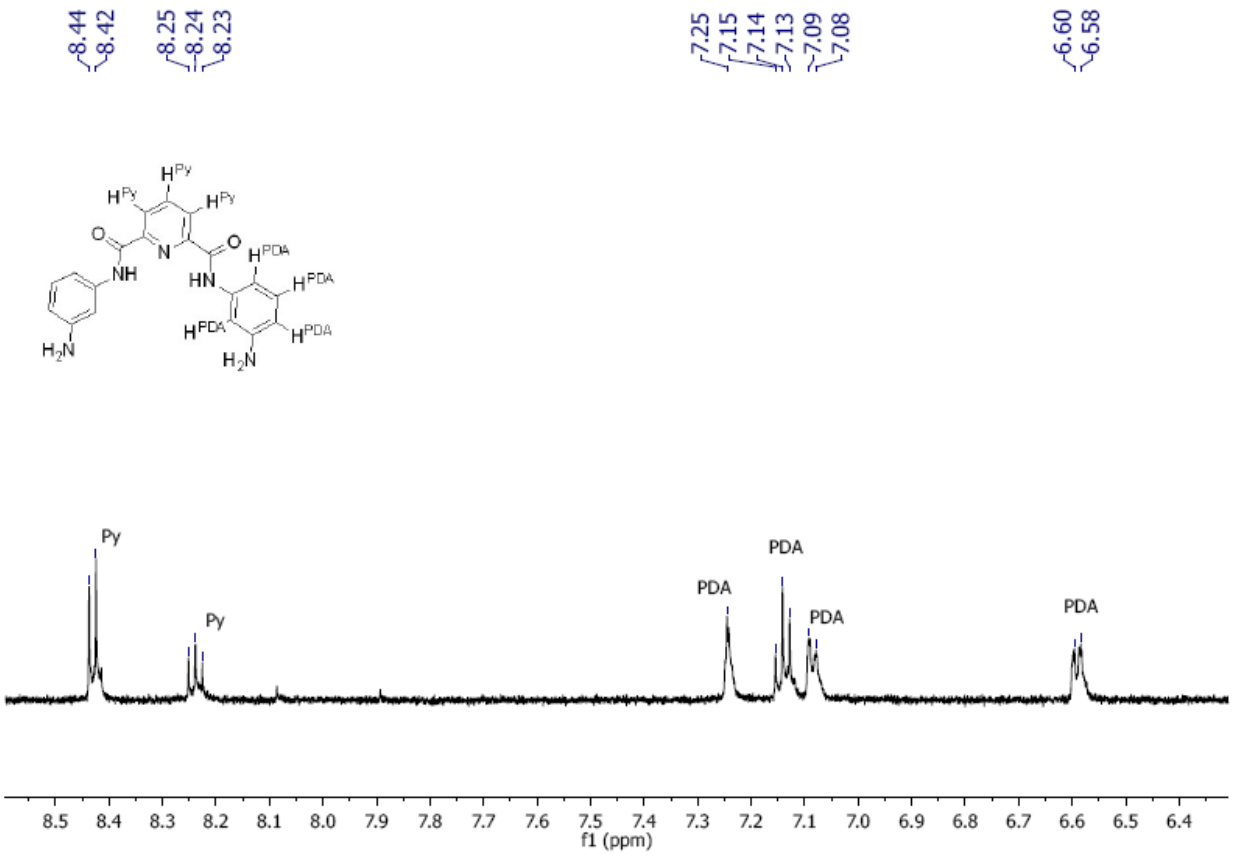
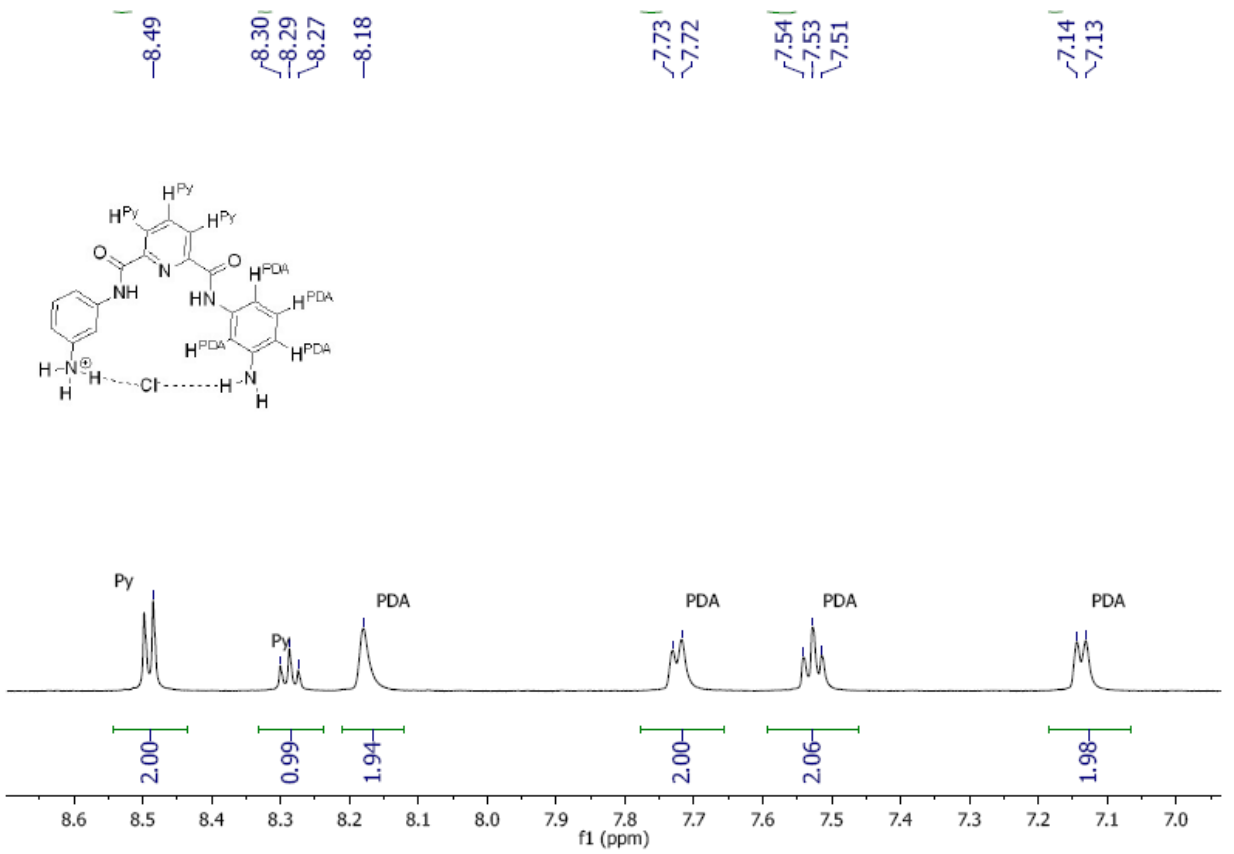
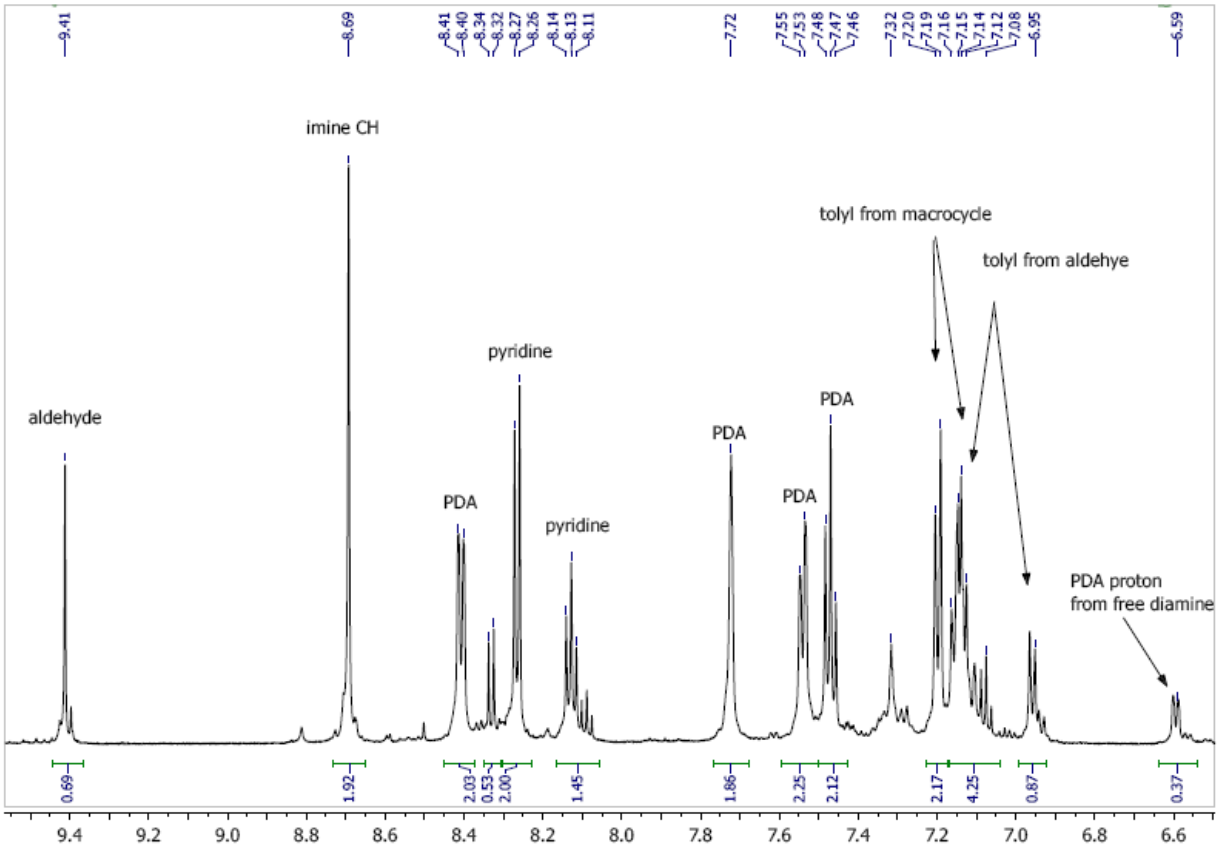



**Figure S16.** Changes of reagent and product concentration during the reaction in the mixture of **1**+**2** and 1 equiv. of HCl aqueous solution. Concentrations of all components were calculated relative to the integral of aldehyde CH proton peak.







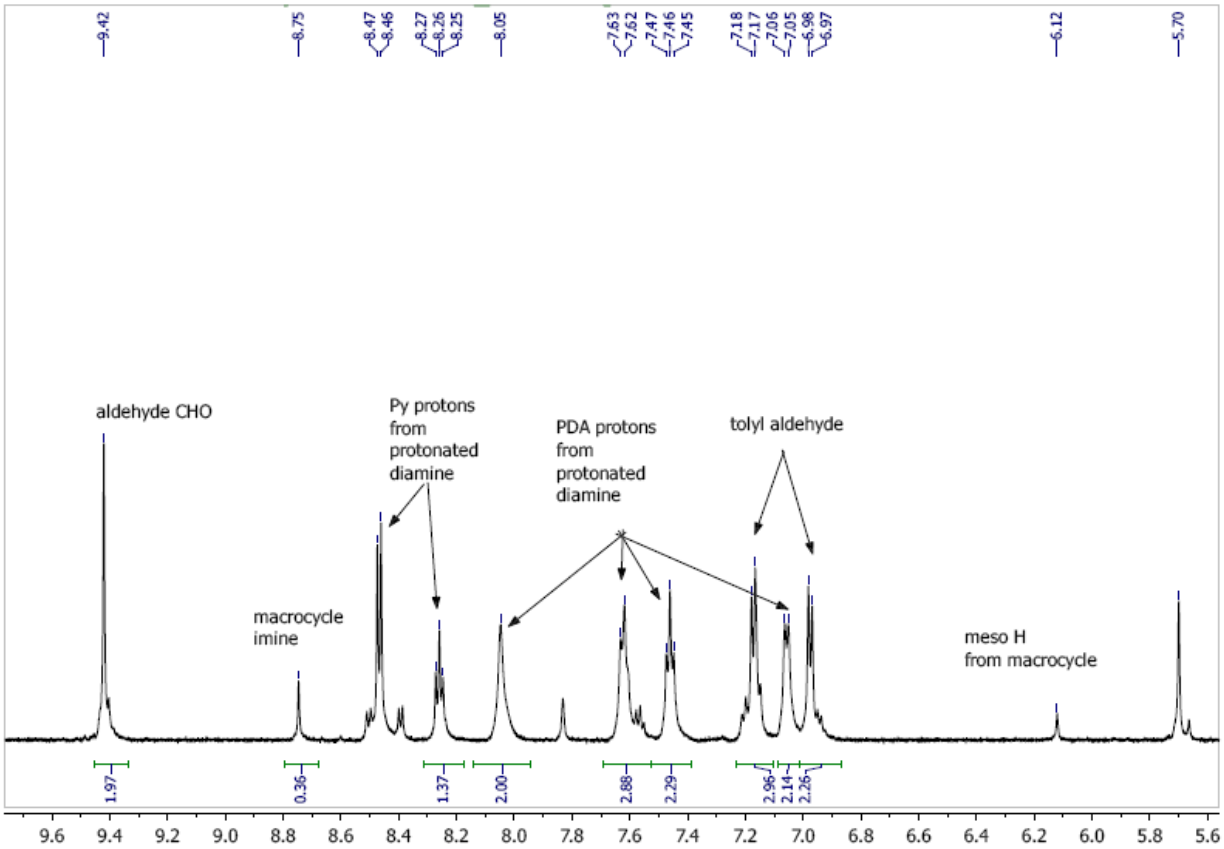



**Figure S17**. Assignment of peaks in the **Figure 3** (see article)

## ESI mass-spectrometry

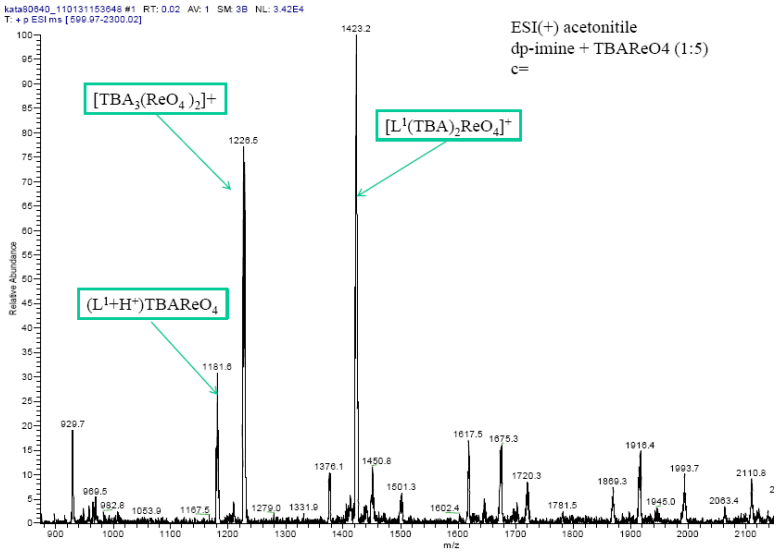



**Figure S18**. ESI(+) of ***L*** $^{1}$ and 5 eq. of $BuN_4ReO_4$ in acetonitrile.

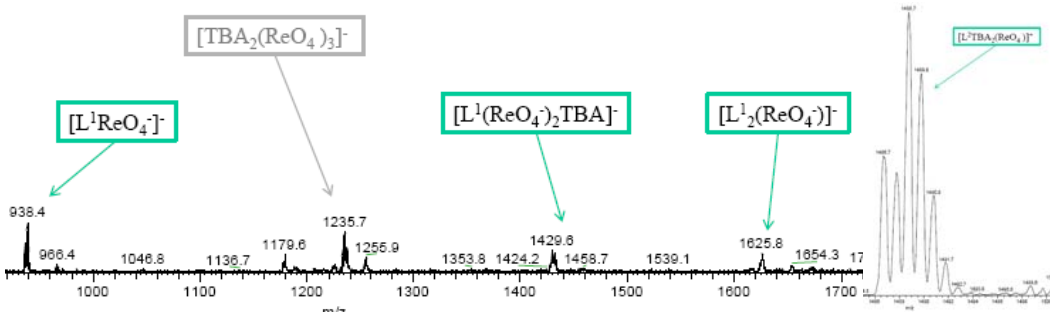



**Figure S19**. ESI(-) of ***L*** $^{1}$ and 5 eq. of $BuN_4ReO_4$ in acetonitrile.

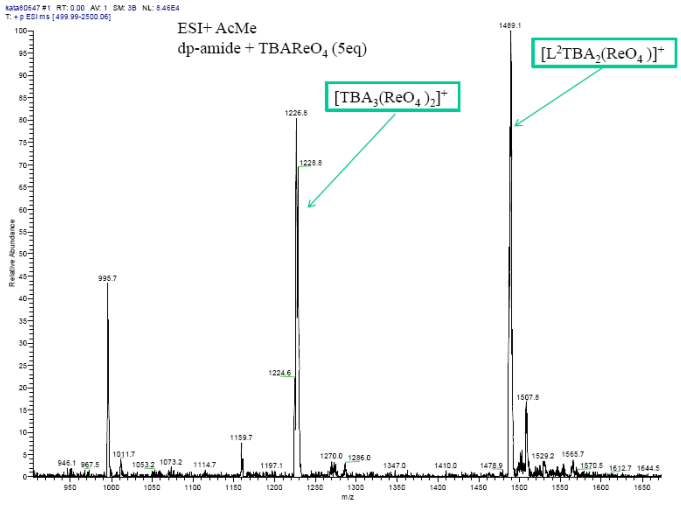



**Figure S20.** ESI (+) of ***L*** $^{2}$ and 5 eq. of $BuN_4ReO_4$ in acetonitrile-DCM 6:1 mixture.

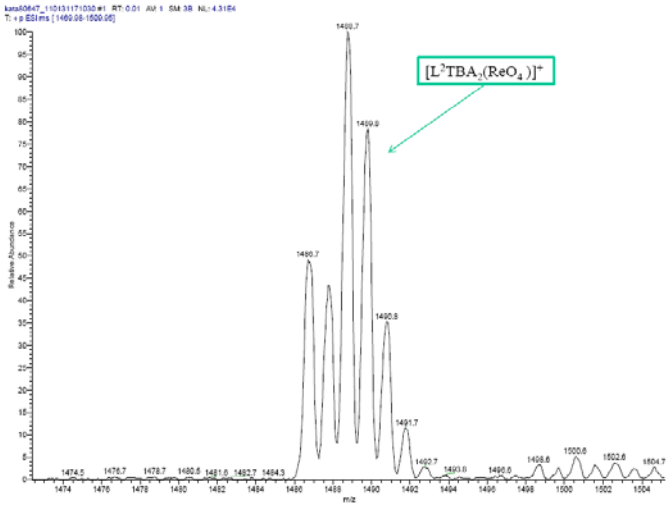



**Figure S21.** ESI (+) of ***L*²** and 5 eq. of $BuN_4ReO_4$ in acetonitrile-DCM 6:1 mixture.

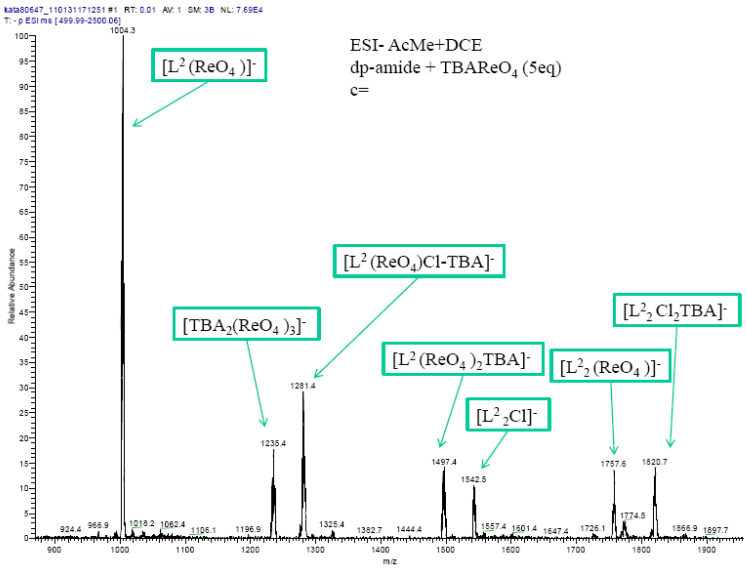



**Figure S22.** ESI (-) of ***L*²** and 5 eq. of $BuN_4ReO_4$ in acetonitrile-DCM 6:1 mixture.

## NMR titration of 2 with different acids

Diamine **2** 4.6 mg (0.08 mmol) was placed in 5 mm NMR tube and 0.6 ml of $CD_3OD$ was added. Then portions of corresponding acids (HCl $_{conc}$ (26%), $HReO_{4\ conc}$ (76%)) were added as their $CD_3OD$ solutions.

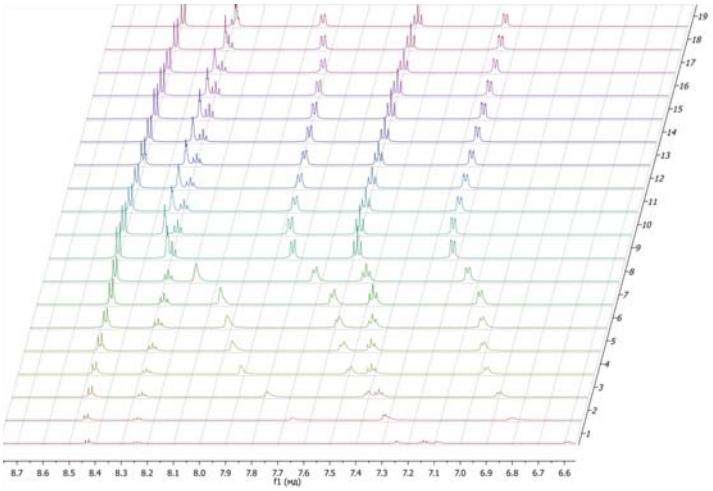


**Figure S23.** $^{1}$H NMR spectra of **2** titration with HCl. 1) before HCl addition; 2) 0.175 eq. HCl; 3) 0.350 eq. HCl 4) 0.525 eq. HCl; 5) 0.700 eq. HCl; 6) 0.875 eq. HCl; 7) 1.050 eq. HCl; 8) 1.225 eq. HCl; 9) 1.400 eq. HCl; 10) 1.575 eq. HCl; 11) 1.750 eq. HCl; 12) 1.925 eq. HCl; 13) 2.100 eq. HCl; 14) 2.275 eq. HCl; 15) 2.450 eq. HCl; 16) 2.950 eq. HCl; 17) 3.500 eq. HCl; 18) 5.835 eq. HCl; 19) 10.5 eq. HCl.

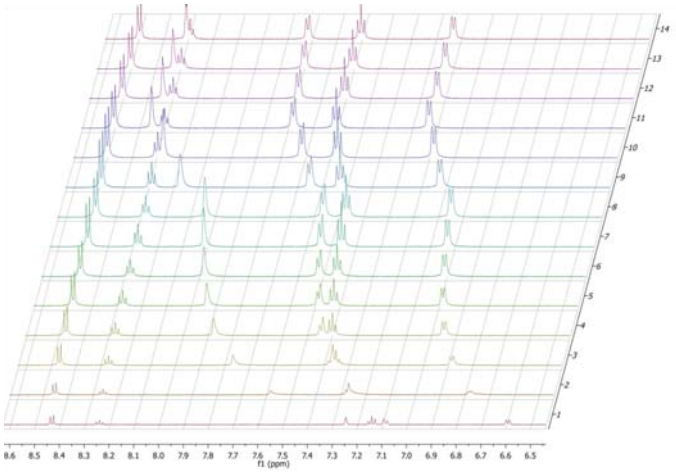


**Figure S24.** $^{1}$H NMR spectra of **2** titration with $HReO_4$. 1) before $HReO_4$ addition; 2) 0.175 eq. $HReO_4$; 3) 0.350 eq. $HReO_4$ 4) 0.525 eq. $HReO_4$; 5) 0.700 eq. $HReO_4$; 6) 0.875 eq. $HReO_4$; 7) 1.050 eq. $HReO_4$; 8) 1.225 eq. $HReO_4$; 9) 1.400 eq. $HReO_4$; 10) 1.575 eq. $HReO_4$; 11) 1.750 eq. $HReO_4$; 12) 1.925 eq. $HReO_4$; 13) 2.100 eq. $HReO_4$; 14) 2.275 eq. $HReO_4$.

## UV-Vis titration[5]

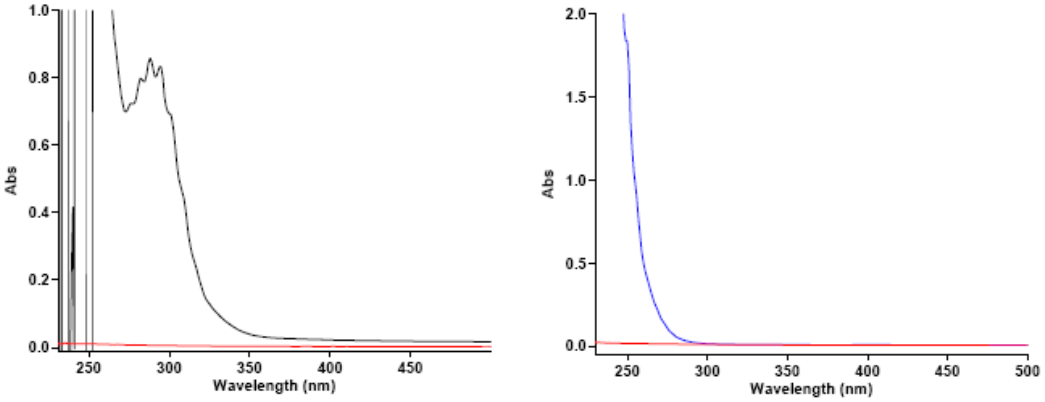
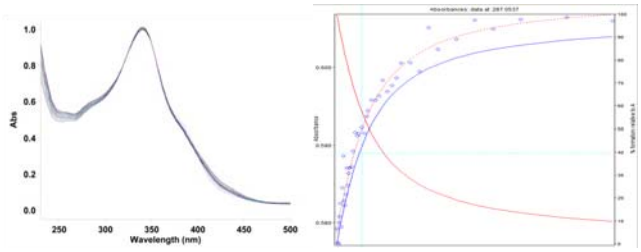



**Figure S25**. UV-vis spectra of $Bu_4NTcO_4$ (left) and $Bu_4NReO_4$ (right) [anion]=$10^{-5}$M.

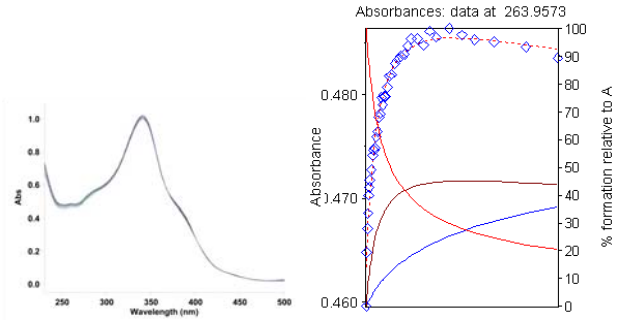
## Titration of L[1] in dichloroethane (DCE)

$TBACl^-$



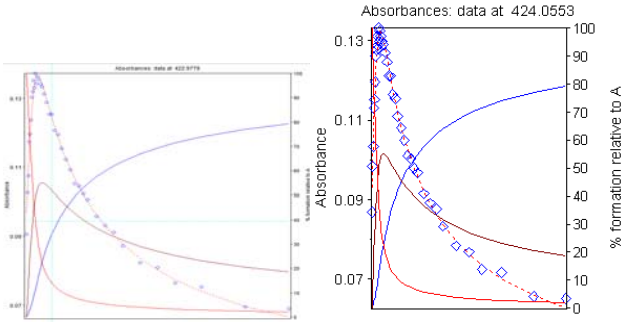
Job plot – complex event which involves stoichiometries 2:1, 1:1 and 1:2

$TBAClO_4$



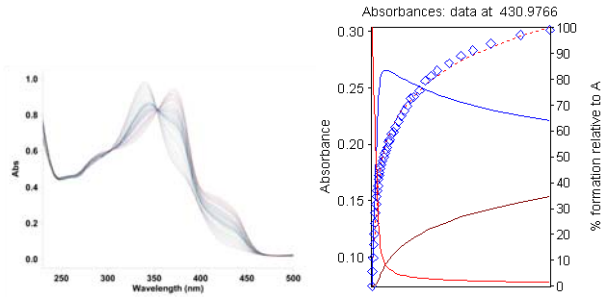

Jop plot 1:1

$TBAH_2PO_4$

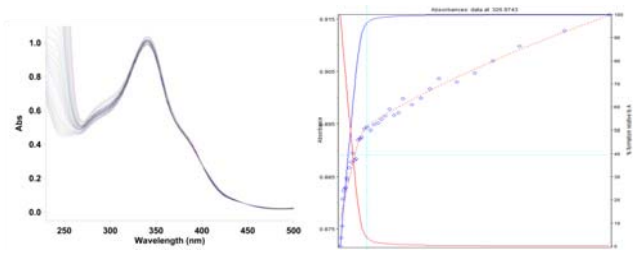



Job plot 1:1

$TBAHSO_4$

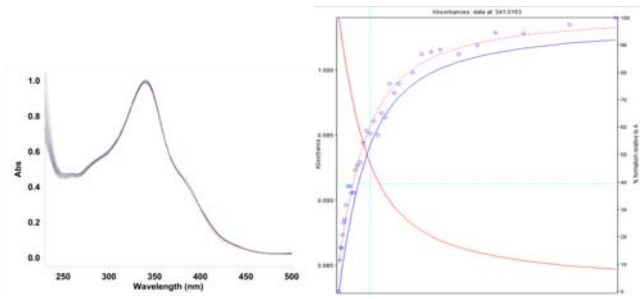



Job plot 1:1



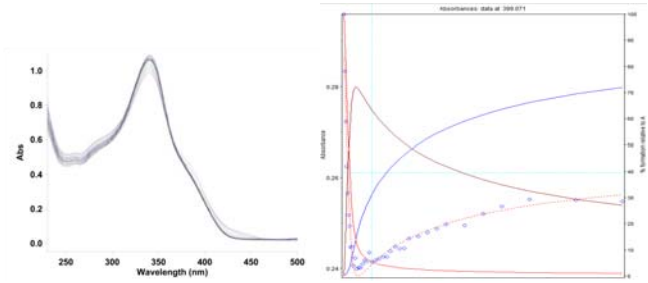

Job plot 1:1

$TBANO_3$



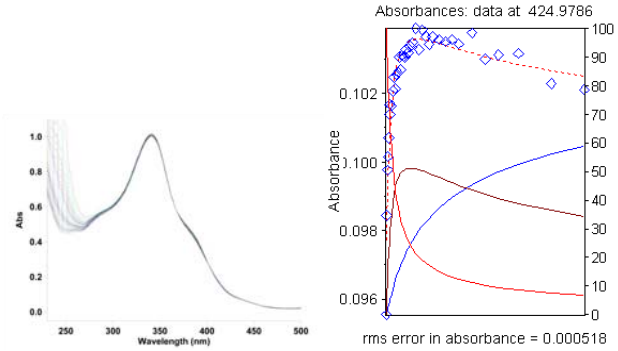

Job plot 1:1

TBAOAc

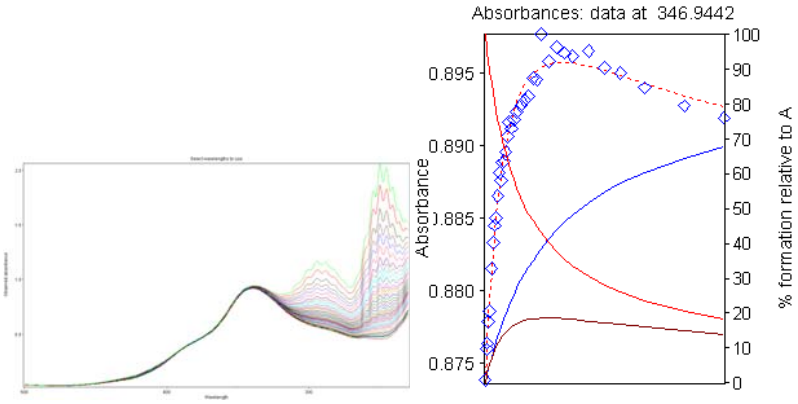



Job plot 1:1

$TBAReO_4$



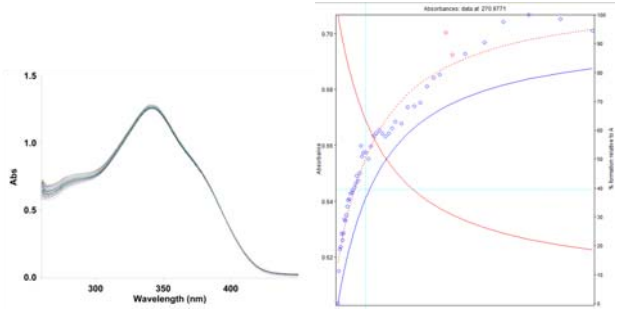

Job plot 1:1



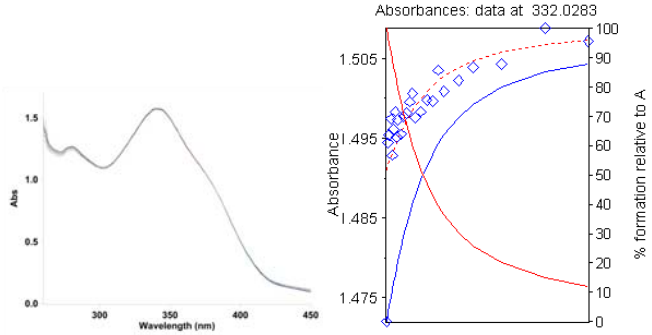

Job plot 1:1

## Titration of $L^1$ in dimethylsulfoxide (DMSO)

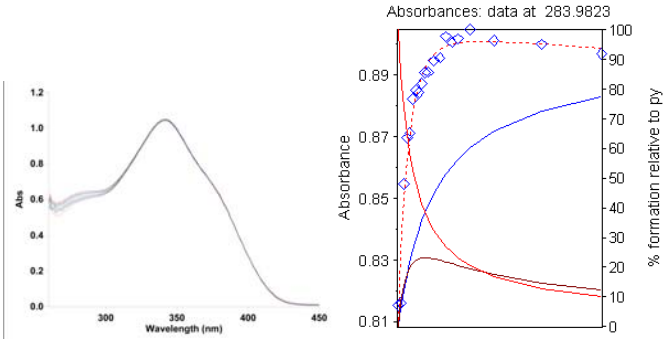
TBACl Job plot was 1:1 for all the anions



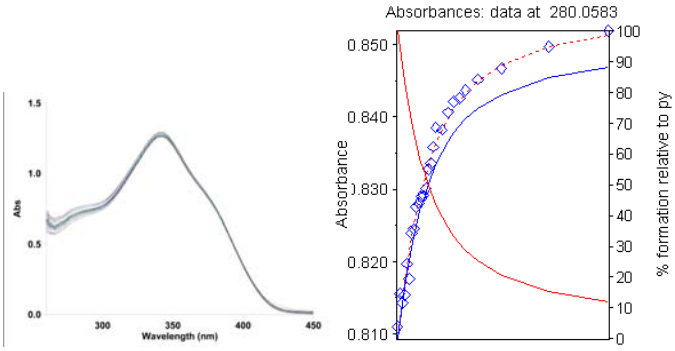
$TBAClO_4$



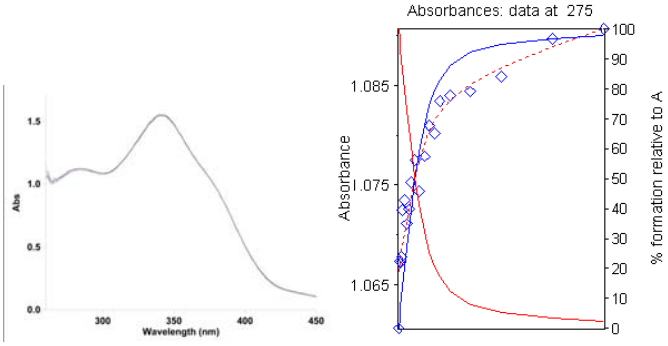
$TBAH_2PO_4$



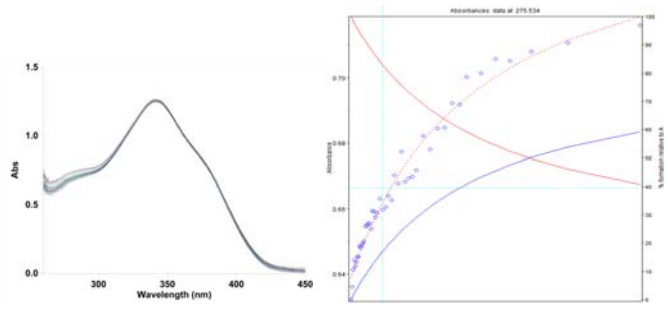

$TBAHSO_4$



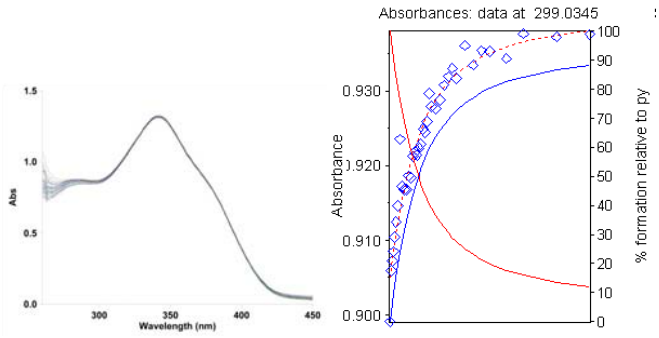

TBAI



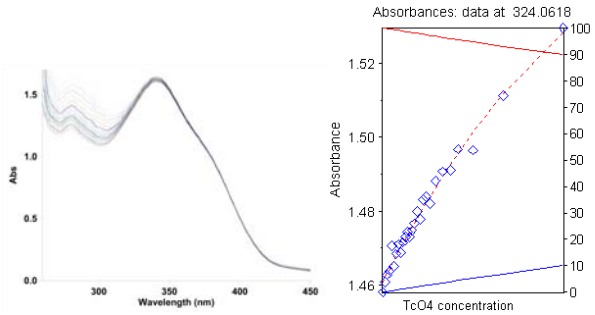

TBAOAc




$TBAReO_4$

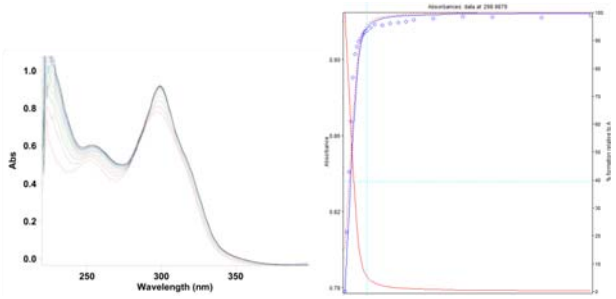



$TBA^{99}TcO_4$

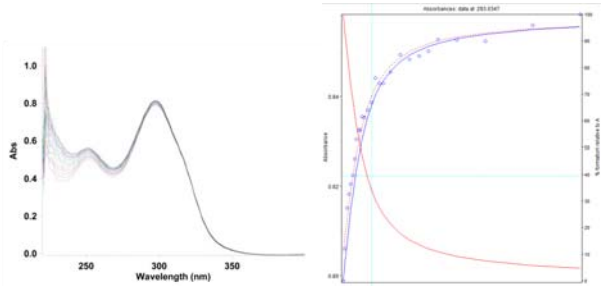



## Titration of $L^2$ in dichloroethane (DCE)

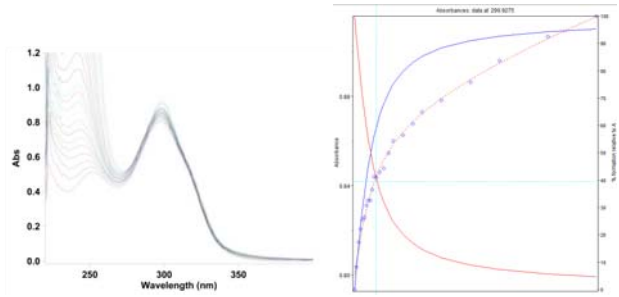
TBACl Job plot was 1:1 for all the anions



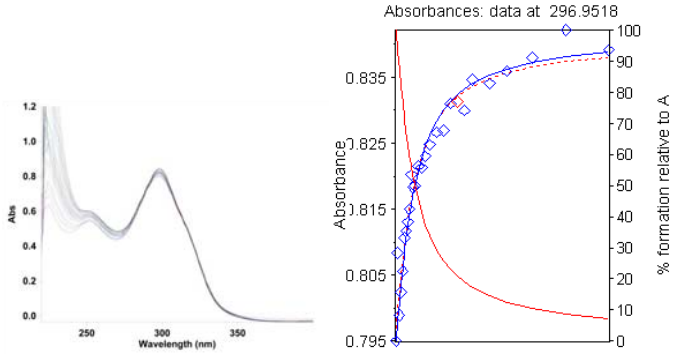

$TBAClO_4$



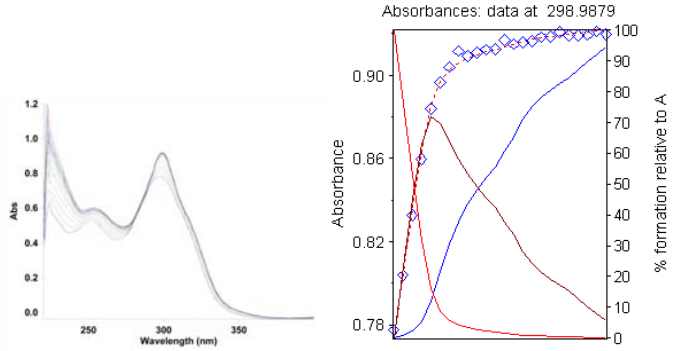

TBAI



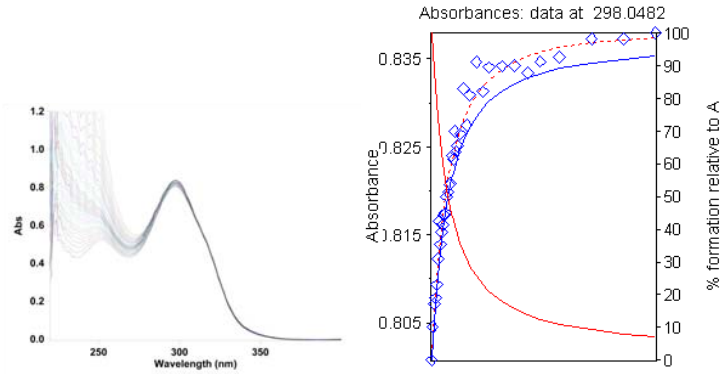

$TBANO_3$



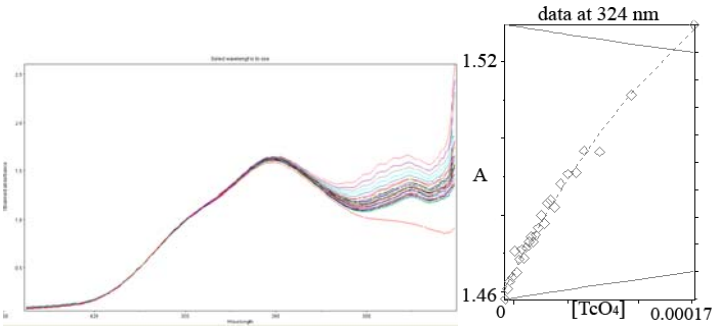

TBAOAc




$TBAReO_4$

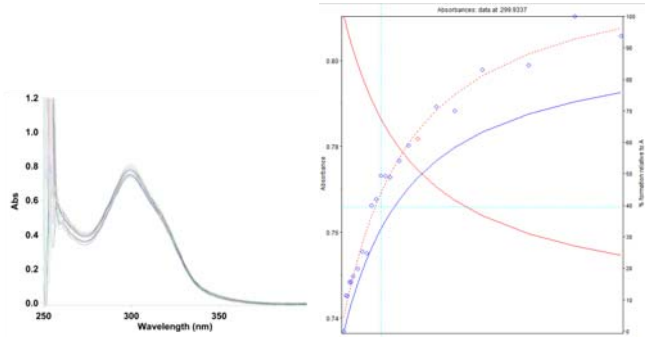



$TBATcO_4$

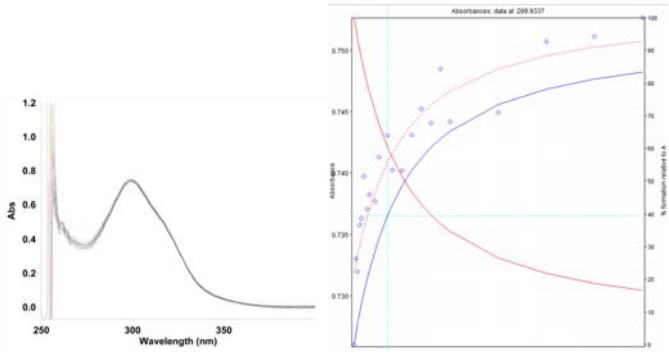



## Titration of L² in dimethylsulfoxide (DMSO)

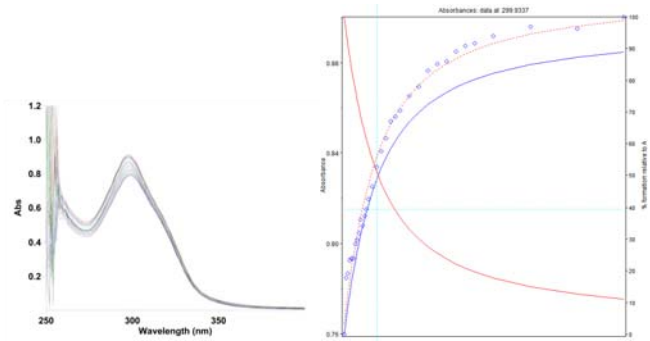
TBACl Job plot was 1:1 for all the anions



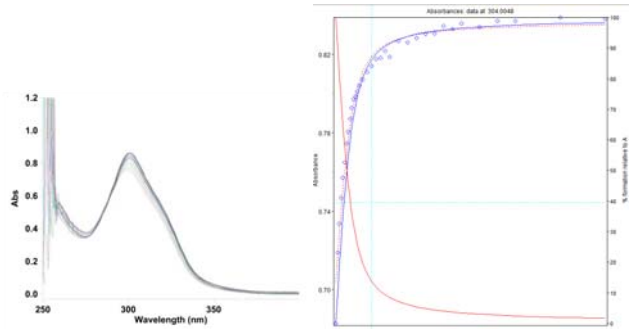

$TBAClO_4$



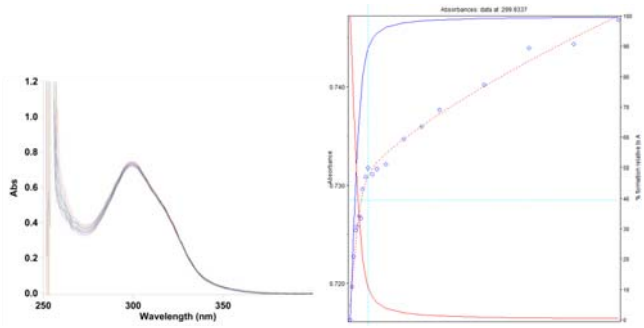

$TBAH_2PO_4$



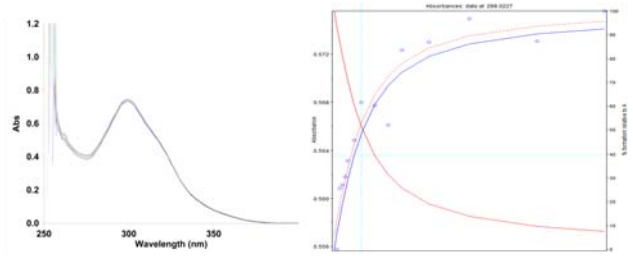
$TBAHSO_4$



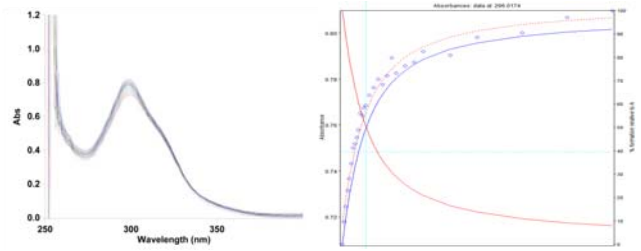

TBAI



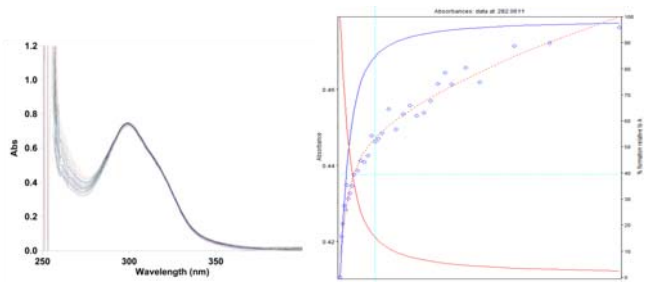

$TBANO_3$



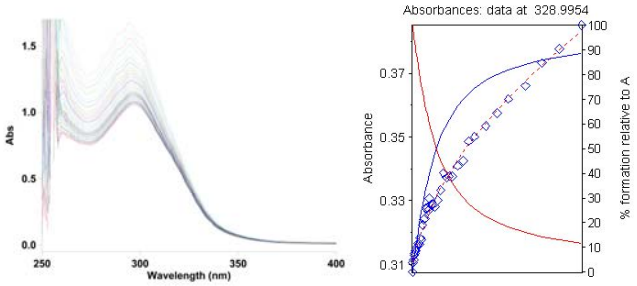

TBAOAc




$TBAReO_4$




$TBA^{99}TcO_4$




## Anion competition experiment

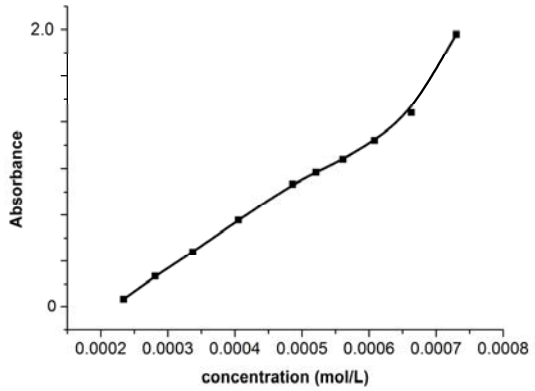



**Figure S26**. Absorbance vs. concentration of ***L*$^{1}$** in DMSO. Starting from concentration 5 × $10^4$ the absorbance does not follow Lambert-Beer behavior.

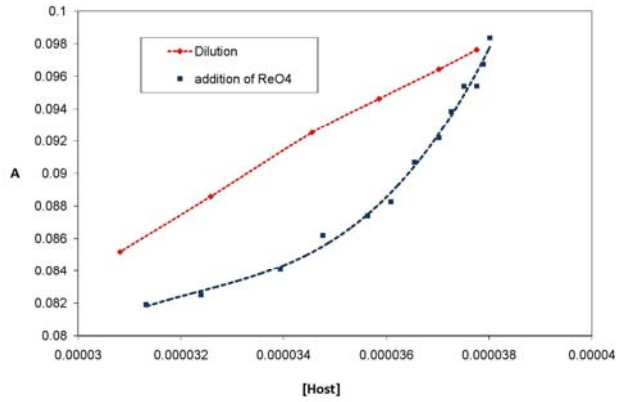



**Figure S27**. Competition experiment in DMSO solution. Changes in the absorbance (at 430 nm) of a mixture of $\boldsymbol{L^1}$+2 equiv. $TBAHSO_4$ upon addition of $\boldsymbol{L^1}$ solution (*i.e.* dilution of the host-guest complex) or a mixture of $\boldsymbol{L^1}$+$TBAReO_4$ (*i.e.* titration with $ReO_4^-$). Fitting of the experimental data using HYPERQUAD Program resulted in competition constant logK = 3.60(2).

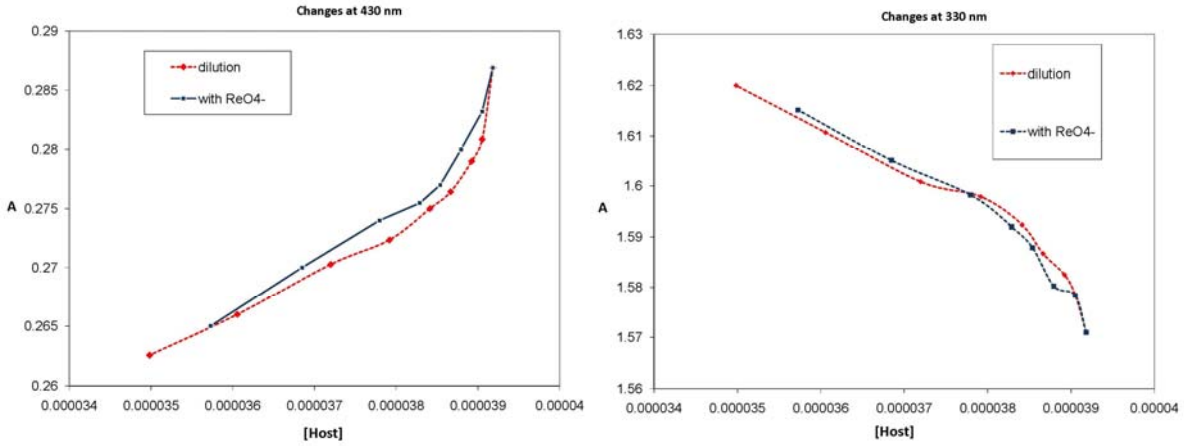



**Figure S28.** Competition experiment in DCE solution. Changes in the absorbance (at 430 and 330 nm) of a mixture of $\boldsymbol{L^1}$+2 equiv. $TBAHSO_4$ upon addition of $\boldsymbol{L^1}$ solution (*i.e.* dilution of host-guest complex) or a mixture of $\boldsymbol{L^1}$+$TBAReO_4$ (*i.e.* titration with $ReO_4^-$).

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