Supplementary Section

Supramolecular receptors in solid phase: developing sensors for anionic radionuclides

Giancarla Alberti[a], Valeria Amendola[a], Greta Bergamaschi[a], Roberta Colleoni[a], Chiara Milanese[a] and Raffaela Biesuz[a]*

[a] *Dipartimento di Chimica – Università di Pavia,via Taramelli 12, 27100 Pavia, Italy. Fax: +39 0382 528544; Tel: +39 0382 9873448; E-mail: rbiesuz@unipv.it*
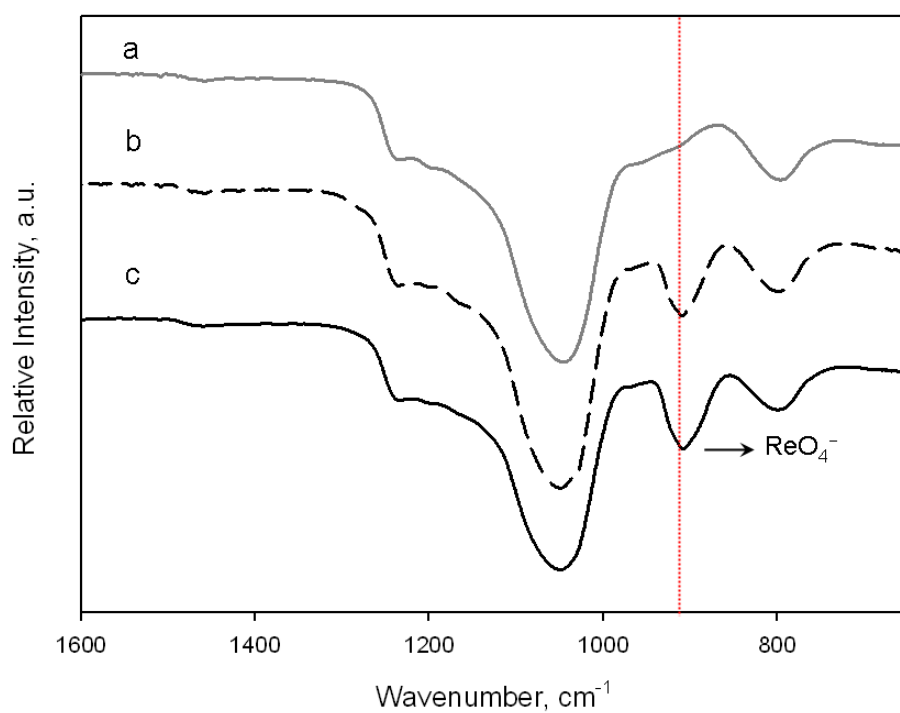
Fig. S1: FT-IR spectra of **s-2**, before (a) and after the treatment with aqueous solutions of $NaReO_4$ at different concentrations (6 and 60 mM, spectra (b) and (c) respectively).

Fig. S2: FT-IR spectra of **a-1**, before (a) and after the treatment with aqueous solutions of $NaReO_4$ at different concentrations (6 and 60 mM, spectra (b) and (c) respectively).
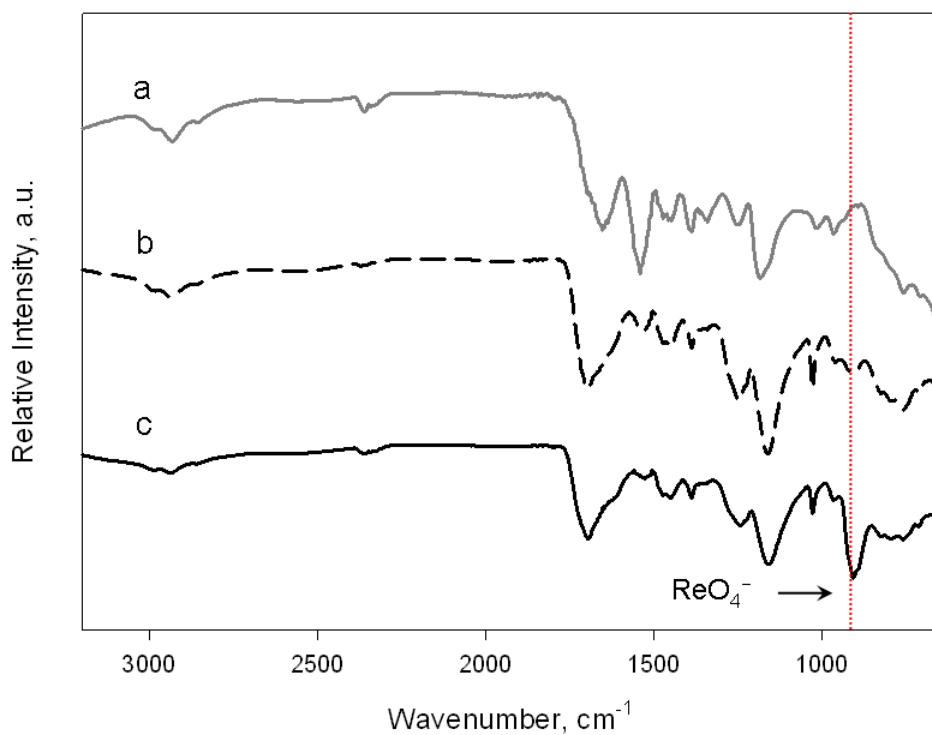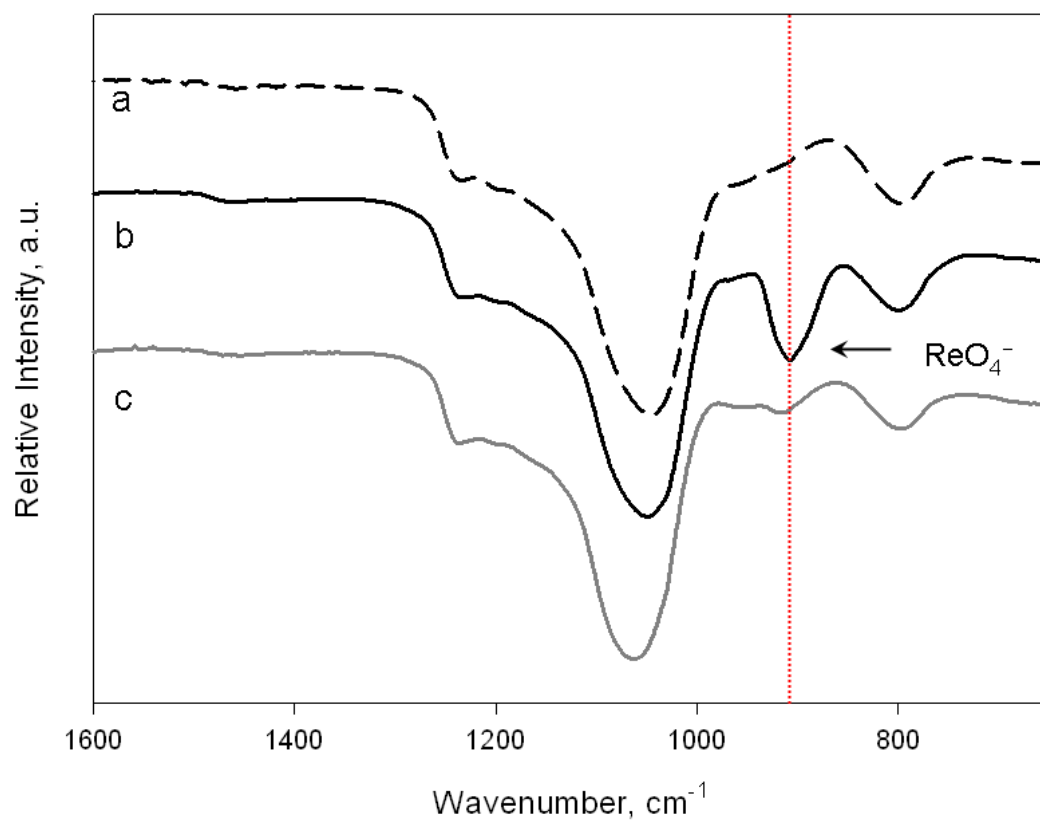
Fig. S3: FT-IR studies of anion exchange: (a) starting material, **s-2** (dashed line); (b) **s-2**–ReO4 obtained from anion exchange of (a) and $NaReO_4$ (black); (c) **s-2** obtained from anion exchange of (b) and NaCl
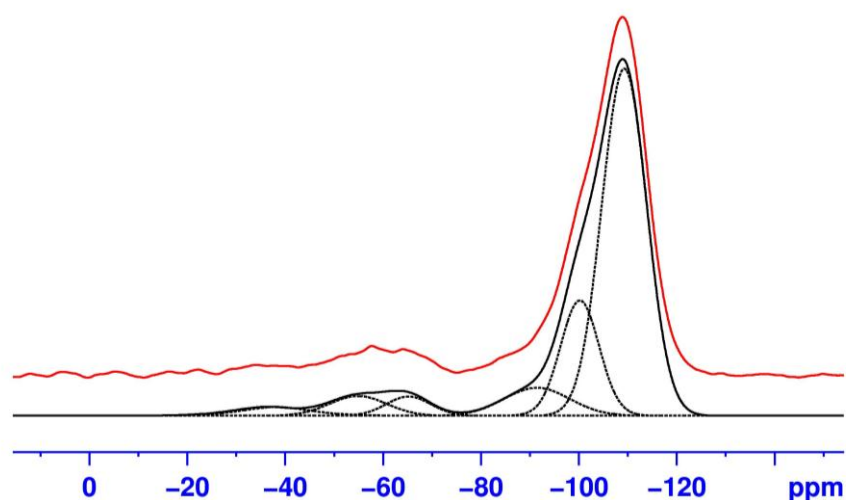
Fig. S4: ^{29}Si MAS NMR spectrum of sample **s-1**: the peaks in the region -90 to -110 ppm are due to the Q^n population (all Si-O bonds), the peaks in the region -40 to -70 ppm are due to the T^n population (Si with at least a Si-C bond). Experimental data red line, simulated single components dotted black lines, total simulated spectrum continuous black line. The characteristics of the peaks are reported in Table S1.

Site	δ_{iso}	LB	xGB / (1-x)LB	In
1	-109.2	861.5	1.0	1
2	-100.1	737.0	0.98	0.29
3	-91.3	1253.1	1.0	0.12
4	-65.1	853.9	1.0	0.05
5	-54.8	1090.8	1.0	0.07
6	-38.0	1296.9	0.6	0.04

Table S1: chemical shift, Lorentzian Broadening, x Guassian Broadening /(1-x)Lorentianz Broadening and integrated area of the deconvoluted peaks of Fig. S4
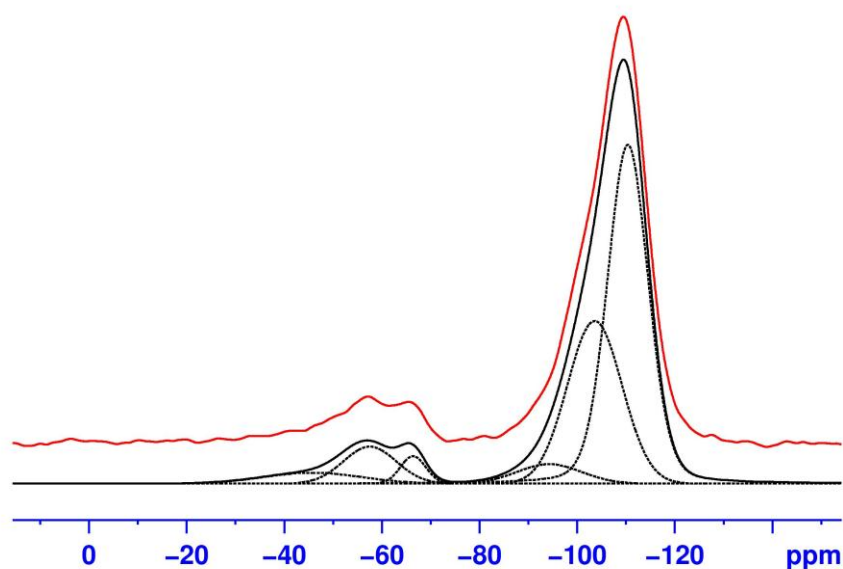
Fig. S5: ^{29}Si MAS NMR spectrum of sample **s-2**: the peaks in the region -90 to -110 ppm are due to the Q^n population (all Si-O bonds), the peaks in the region -40 to -70 ppm are due to the T^n population (Si with at least a Si-C bond). Experimental data red line, simulated single components dotted black lines, total simulated spectrum continuous black line. The characteristics of the peaks are reported in Table S2.

Site	δ_{iso}	LB	xGB / (1-x)LB	In
1	-110.3	783	0.8	1
2	-103.5	1048	1	0.59
3	-94.2	1236	1	0.08
4	-66.3	484	1	0.05
5	-57.4	1010	1	0.13
6	-45.7	1870	1	0.07

Table S2: chemical shift, Lorentzian Broadening, x Guassian Broadening /(1-x)Lorentianz Broadening and integrated area of the deconvoluted peaks of Fig. S5.
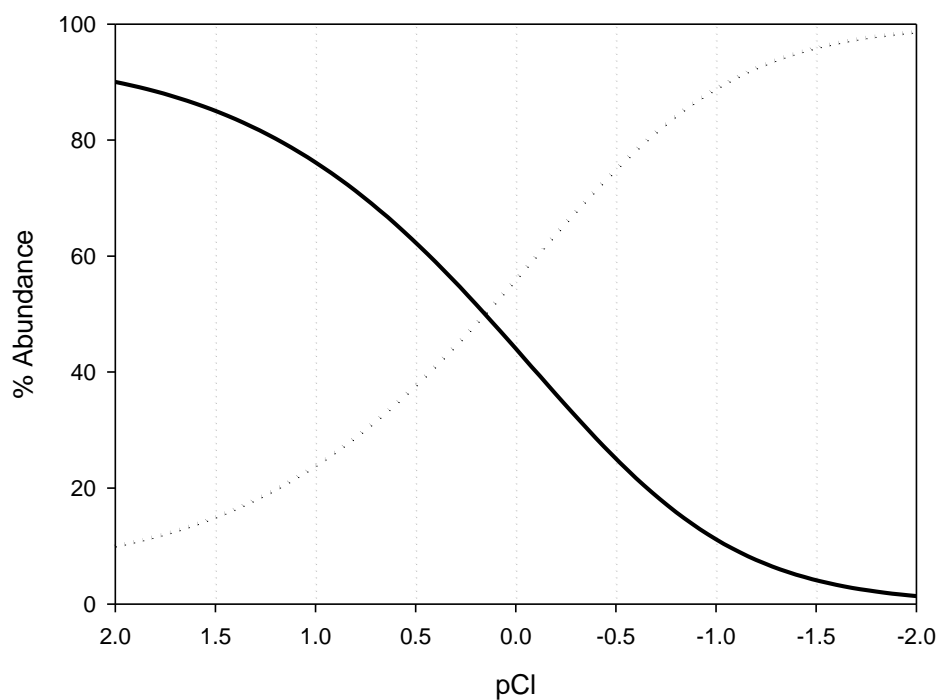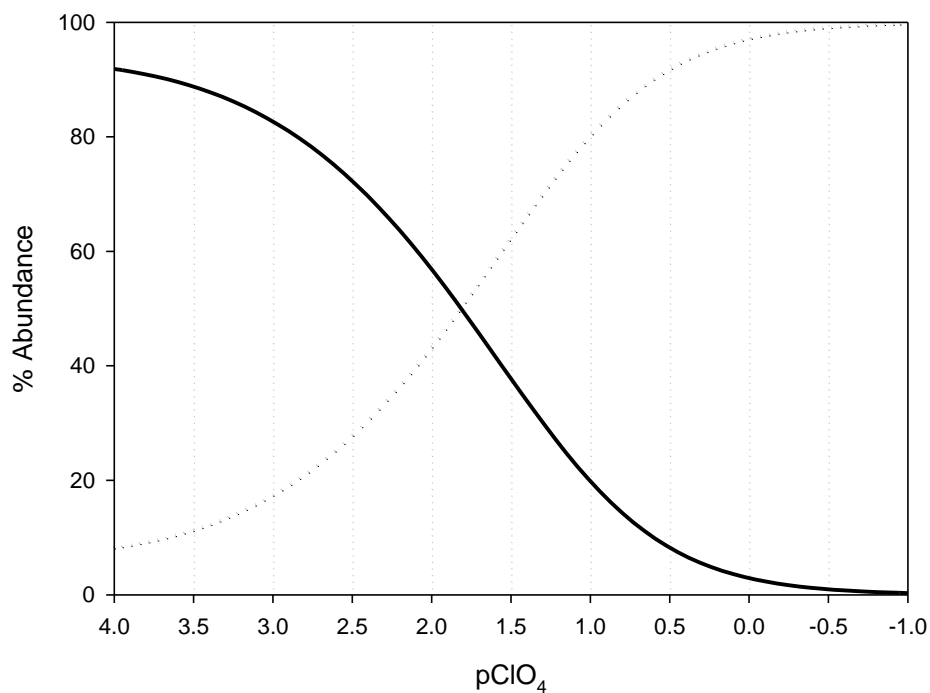
Fig. S6 (a)

Fig. S6 (b)

Hyss output of competition of chloride Fig. S6(a) and perchlorate Fig. S6(b). The affinity constants found for the azacryptand in solution[5] have been used, assuming that $c_{ReO4^-} = c_{azacrip} = 0.0017$ M (i.d referred to the solution volume, $V=10$ mL, considering the capacity of the cage, $q= 0.35$ mmol/g, and the amount of solid, 50 mg). To have 90% of free ReO_4^- in solution, the total anion concentration was calculated equal to 11.5 M in the case of chloride, 0.26 M in the case of perchlorate (solid line: **s-1**(ReO_4) adduct; dotted line: free perrhenate).