Allosteric effects in norbadione A. A clue for the accumulation process of ^{137}Cs in mushrooms?

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Supplementary Data

6 pages

Table S1 ^{1}H Chemical shifts (ppm *vs* TMS), multiplicity and coupling constants (Hz) of norbadione A (1.47×10^{-2} M) solutions as a function of pD. Solvent: CD_3OD/D_2O (80/20 by weight), T = 25.0(2) °C.

proton	pD = 1.0	pD = 2.1	pD = 3.4	pD = 6.4	pD = 8.5	pD = 10.0
3	7.51 (s)	7.48 (s)	7.43 (d, 0.9)	7.41 (s)	7.41 (s)	7.32 (s)
5	8.98 (s)	9.07 (d, 0.9)	9.09 (d, 0.9)	9.11 (d, 0.8)	9.11 (s)	9.10 (s)
7	8.93 (s)	9.00 (d, 0.9)	9.02 (d, 0.9)	9.04 (d, 0.5)	9.04 (s)	9.00 (s)
8, 8'	7.41 (d, 8.8)	7.36 (d, 8.7)	7.29 (d, 8.7)	7.27 (d, 8.4)	7.32 (br)	7.56 (br)
9, 9'	6.96 (d, 8.5)	6.95 (d, 8.8)	6.92 (d, 9.0)	6.90 (d, 8.8)	6.91 (d, 8.8)	6.90 (d, 8.8)
8'', 8'''	7.30 (d, 8.6)	7.26 (d, 8.7)	7.22 (d, 8.7)	7.22 (d, 8.3)	7.32 (br)	7.56 (br)
9'', 9'''	6.93 (d, 8.5)	6.92 (d, 8.7)	6.90 (d, 9.0)	6.88 (d, 8.8)	6.89 (d, 9.2)	6.87 (d, 8.9)

br =broad signal

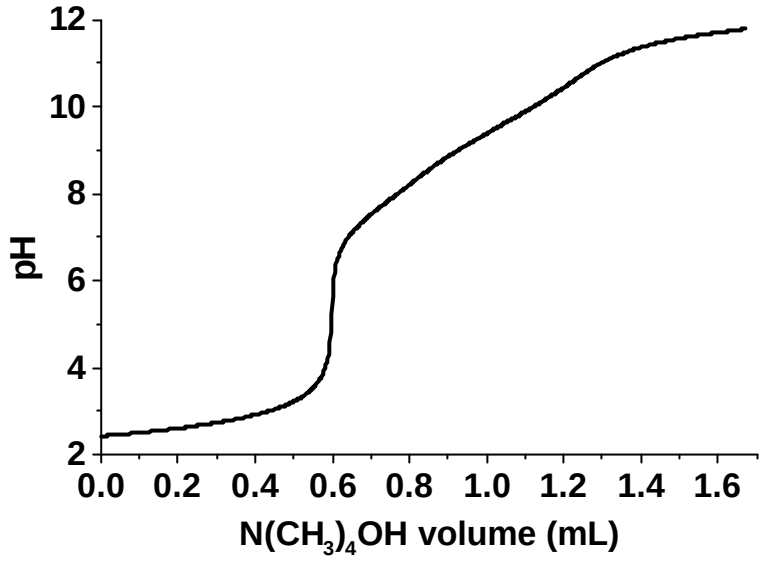

Figure S1 Potentiometric titration of norbadione A (1.50×10^{-3} M) by $N(CH_3)_4OH$ (1.03×10^{-1} M). Solvent: methanol/water (80/20 by weight); T = 25.0(2) °C; I = 0.1 M ($N(C_2H_5)_4ClO_4$).

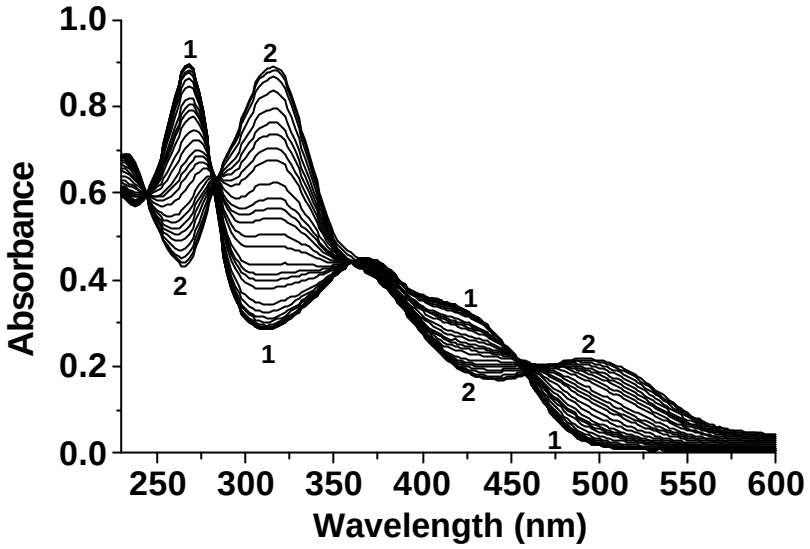

Figure S2 Absorption spectra of norbadione A (1.90×10^{-5} M) as a function of pH. Solvent: methanol/water (80/20 by weight); T = 25.0(2) °C; I = 0.1 M ($N(C_2H_5)_4ClO_4$); l = 1 cm. Spectra: (1) pH = 4.86; (2) pH = 10.40.

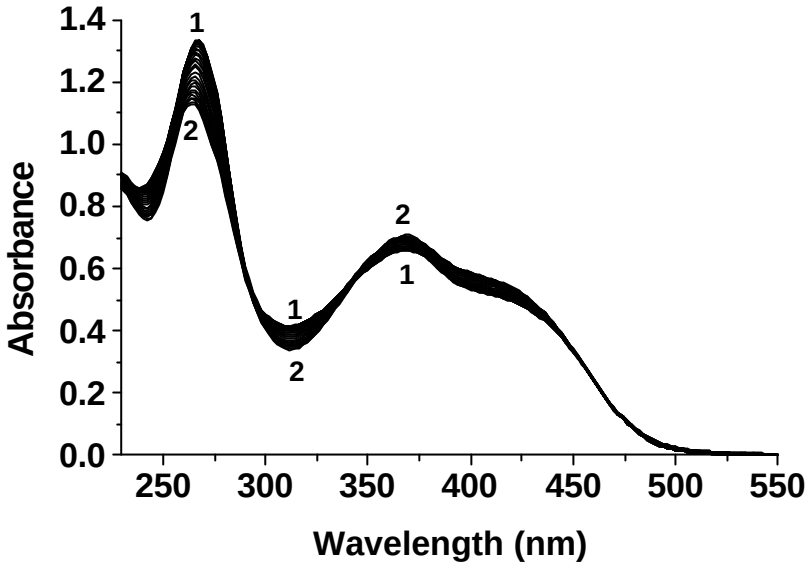

Figure S3 Absorption spectra of norbadione A (2.38×10^{-5} M) as a function of pH. Solvent: methanol/water (80/20 by weight); T = 25.0(2) °C; I = 0.1 M ($N(C_2H_5)_4ClO_4$); l = 1 cm. Spectra: (1) pH = 3.63; (2) pH = 1.05.

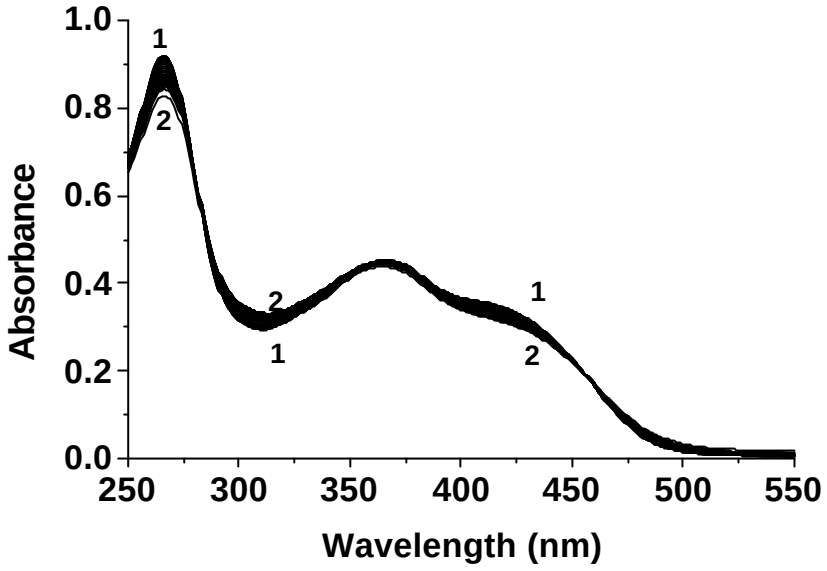

Figure S4 Spectrophotometric titration of norbadione A (9.89×10^{-6} M) by cæsium. Solvent: methanol/water (80/20 by weight); T = 25.0(2) °C; 0.1 M succinic acid/TMAOH buffer; pH = 6.1; l = 2 cm; Spectra (1) $[Cs^+] = 0$; (2) $[Cs^+]_{tot} = 1.02 \times 10^{-4}$ M.