

Supporting Information for

## A comparative evaluation of calix[4]arene-1,3-crown-6 as a ligand for selected divalent cations of radiopharmaceutical interest

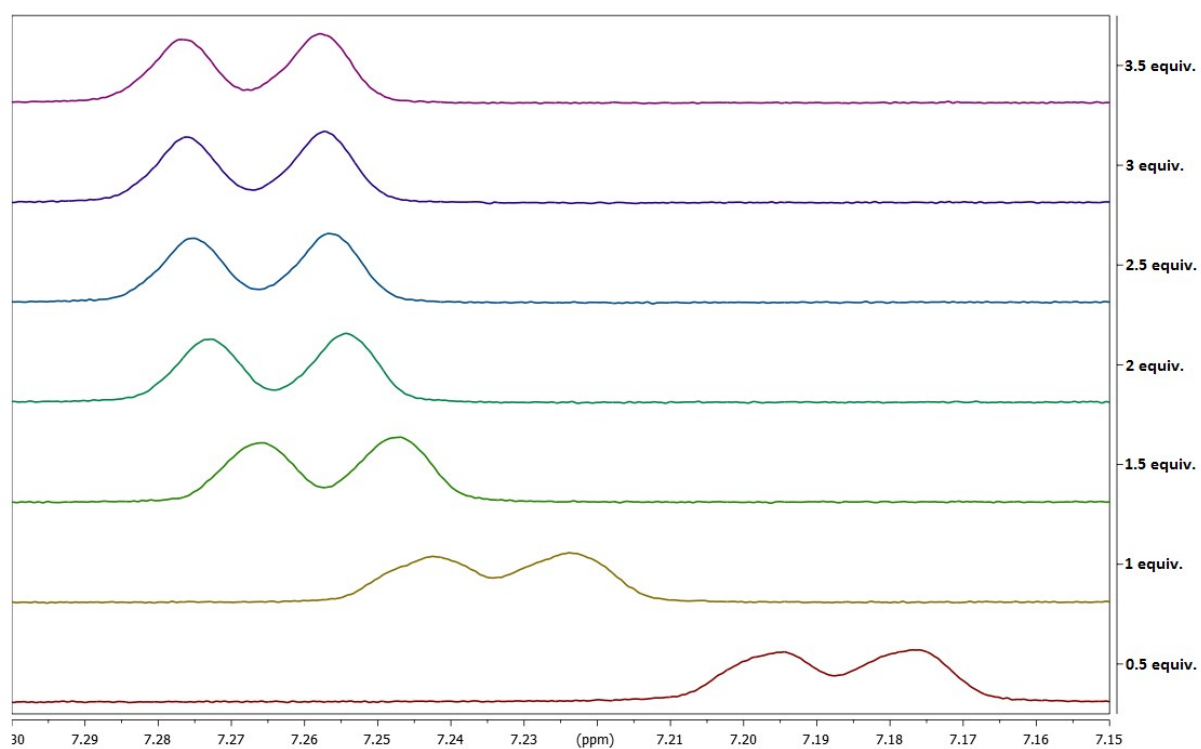
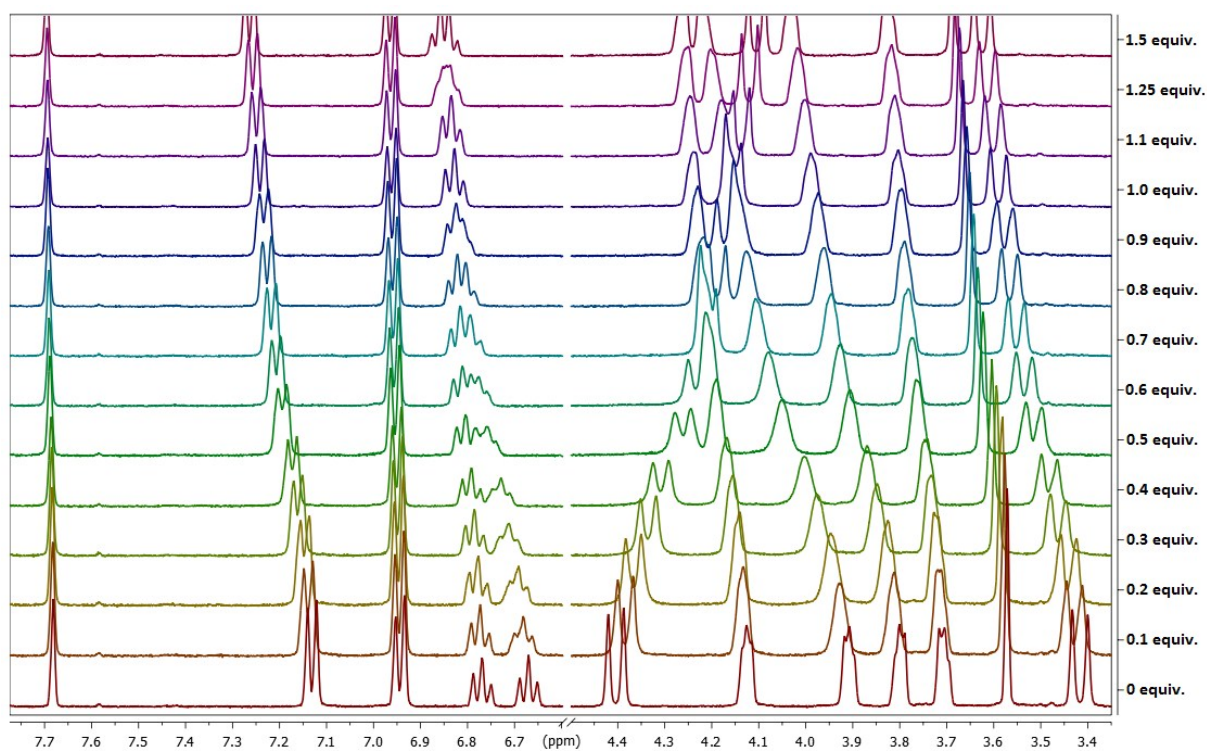
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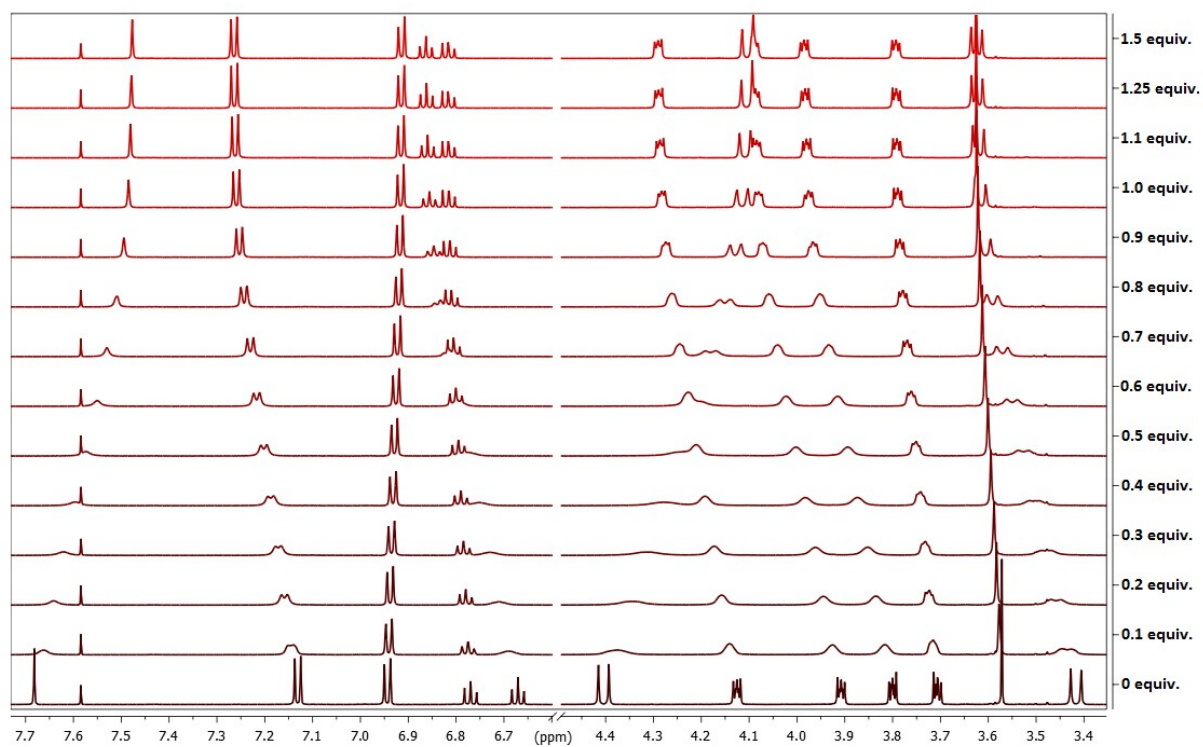
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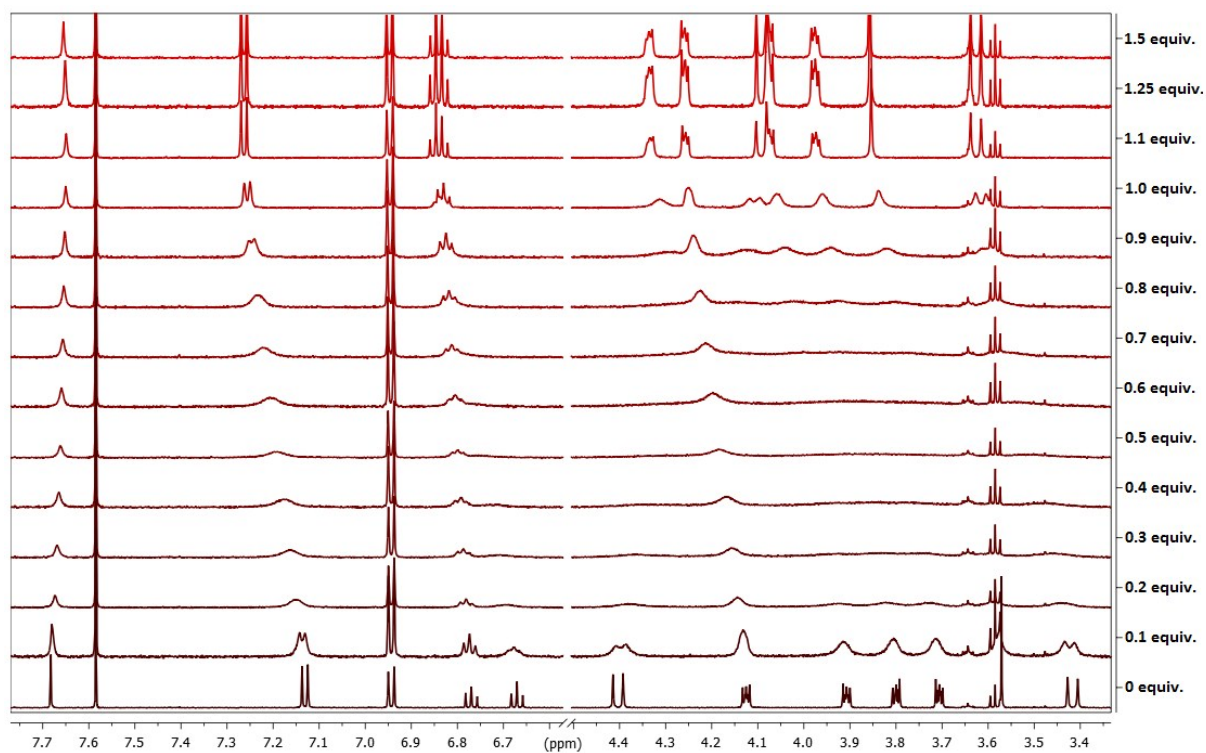
NMR titration experiment of calix **1** with Sr<sup>2+</sup>



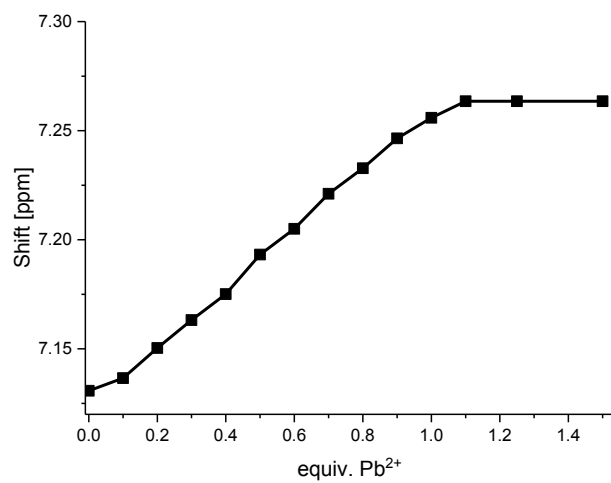
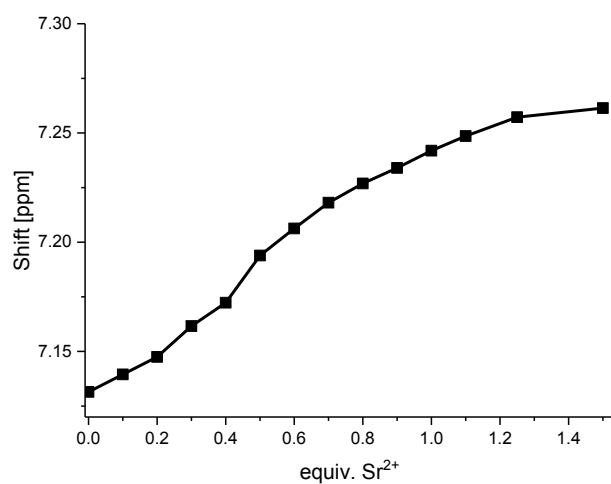
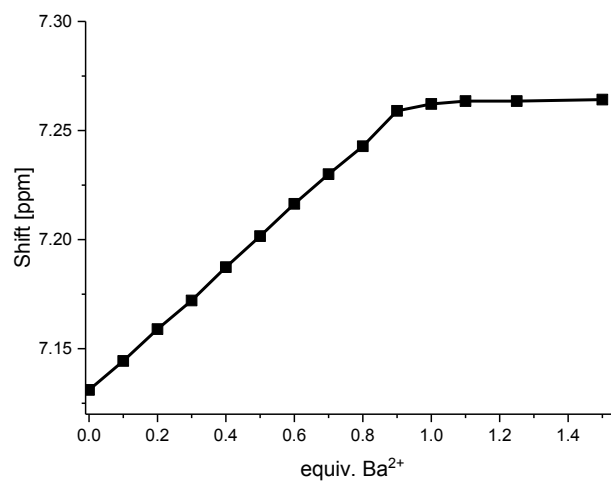
NMR titration experiment of calix **1** with Ba<sup>2+</sup>



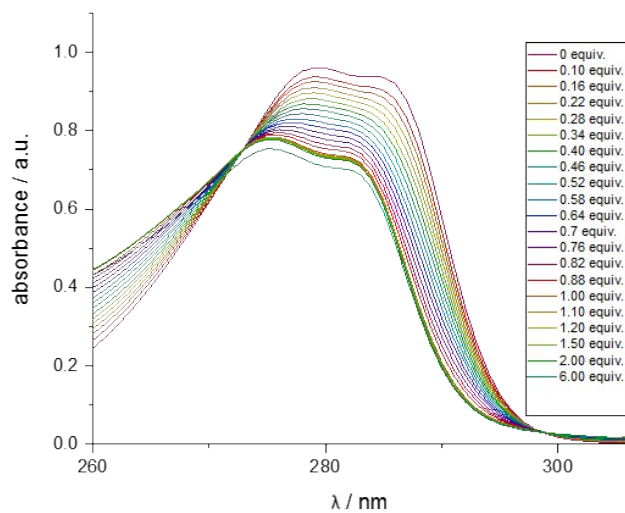
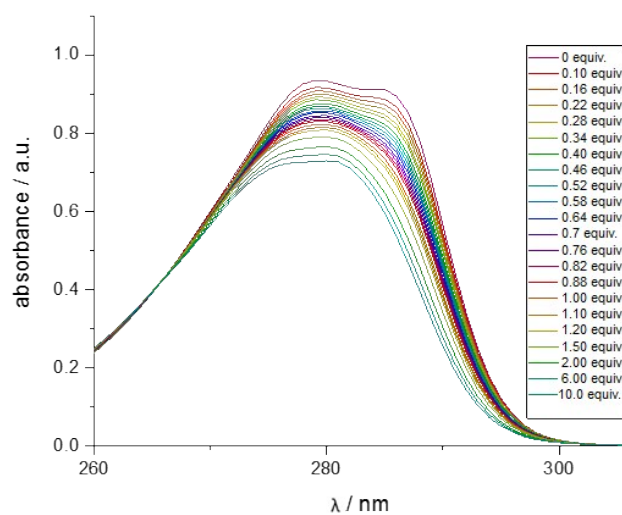
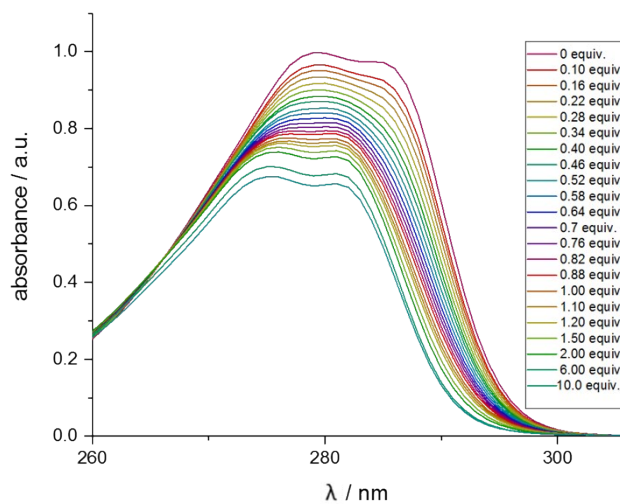
NMR titration experiment of calix **1** with Pb<sup>2+</sup>



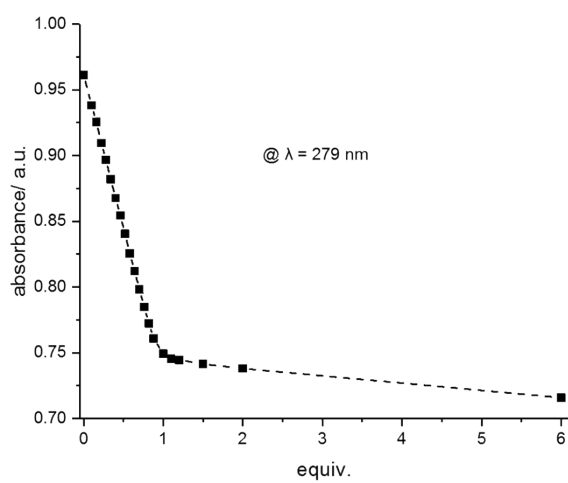
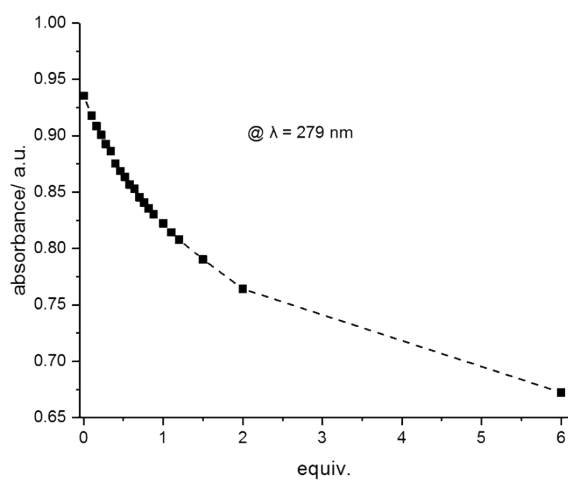
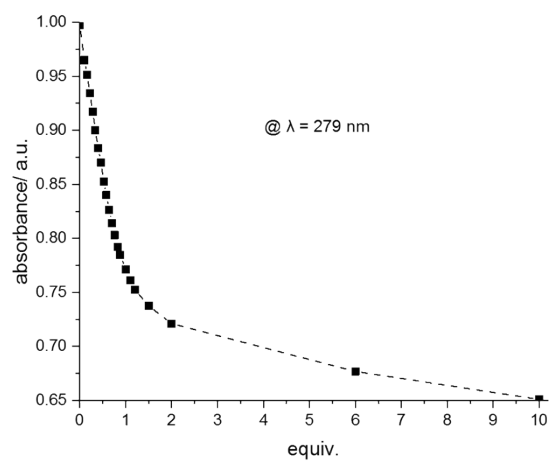
NMR titration plots of calix **1** with Ba<sup>2+</sup>, Sr<sup>2+</sup>, and Pb<sup>2+</sup>



UV/Vis titration experiment of calix **1** with Ba<sup>2+</sup>, Sr<sup>2+</sup>, Pb<sup>2+</sup>



UV/Vis titration plots of calix ligand **1** with Ba<sup>2+</sup>, Sr<sup>2+</sup>, and Pb<sup>2+</sup>



## Crystal data for ligand 1

<b>Crystal data</b>	
<b>Chemical formula</b>	C <sub>78</sub> H <sub>86</sub> Cl <sub>4</sub> O <sub>16</sub>
<b>Mr</b>	1421.26
<b>Crystal system, space group</b>	Monoclinic, <i>P2/n</i>
<b>Temperature (K)</b>	123
<b><i>a</i>, <i>b</i>, <i>c</i> (Å)</b>	10.0307 (3), 14.0336 (5), 12.5626 (4)
<b><math>\beta</math> (°)</b>	100.105 (1)
<b><i>V</i> (Å<sup>3</sup>)</b>	1741.0 (1)
<b><i>Z</i></b>	1
<b>Radiation type</b>	Mo <i>K</i> $\alpha$
<b><math>\mu</math> (mm<sup>-1</sup>)</b>	0.24
<b>Crystal size (mm)</b>	0.15 × 0.13 × 0.13
<b>Data collection</b>	
<b>Diffractometer</b>	Bruker APEX-II CCD
<b>Absorption correction</b>	Multi-scan Bruker-Nonius SADABS
<b>No. of measured, independent and observed [<i>I</i> &gt; 2<math>\sigma</math>(<i>I</i>)] reflections</b>	22332, 6567, 5055
<b><i>R</i><sub>int</sub></b>	0.035
<b>(<i>sin</i> <math>\theta</math>/<math>\lambda</math>)<sub>max</sub> (Å<sup>-1</sup>)</b>	0.770
<b>Refinement</b>	
<b><i>R</i>[<i>F</i><sup>2</sup> &gt; 2<math>\sigma</math>(<i>F</i><sup>2</sup>)], <i>wR</i>(<i>F</i><sup>2</sup>), <i>S</i></b>	0.046, 0.125, 1.03
<b>No. of reflections</b>	6567
<b>No. of parameters</b>	264
<b>H-atom treatment</b>	H-atom parameters constrained
<b><math>\Delta\rho_{\text{max}}</math>, <math>\Delta\rho_{\text{min}}</math> (e Å<sup>-3</sup>)</b>	0.45, -0.36

Computer programs: Bruker APEX2, Bruker SAINT, SHELXS2014 (Sheldrick, 2014), SHELXL2014 (Sheldrick, 2014), Bruker SHELXTL.