Supporting information for :

Harnessing medically-relevant Metals onto water-soluble Subphthalocyanines: towards Bimodal Imaging and Theranostics

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A. CHEMISTRY

For clarity purposes simple labels are used all along the manuscript text:

- Subphthalocyanine (**SubPc**) with a distal phenoxy picket are labelled according to the substituent in para position: **SubPc-DOTA** (**1**), **SubPc-DTPA** (**2**), **SubPc-MDOTA** (**1-M**), **SubPc-MDTPA** (**2-M**).

A.1. Chemicals

Chemicals used in this study are from various providers: Acros Organics [1,2-dicyanobenzene (98 %, ref. 174012500), 4-nitrophenol (99 %, ref. 157052500), gadolinium (III) nitrate pentahydrate (99.9 %, ref. 199140250), copper (II) nitrate trihydrate (99 %, 207680025)], Sigma Aldrich [boron trichloride (1 M in p-xylene, 345458), 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (≥ 99 %, P4329), lutethium (III) chloride hexahydrate (99.9 %, ref. 298131)], Alfa Aesar [palladium 10 % on carbon (A12012), trifluoroacetic acid (99 %, A12198), indium (III) chloride anhydrous (99.9 %, 41977), gallium (III) chloride anhydrous (99.99 %, 11867)], Chematech [2-(4,7,10-tris(2-(tert-butoxy)-2-oxoethyl)-1,4,7,10-tetraazacyclododecan-1-yl)acetic acid (≥ 98 %,C060)] Strem Chemicals [yttrium chloride hexahydrate (99.9 %, ref. 93-3903)]. All chemicals and solvents were used as supplied without further purification.

A.2. Chromatography

Compounds **3**, **4**, **5** and **6** were purified on column chromatography using silica gel (60A, SDS) and a specific mixture of solvent as described in full text. Compound **3** was purified on column chromatography using alumina gel (60A, SDS) and a specific mixture of solvent as described in full text.

B. ANALYSIS

B.1. SubPc-DOTA (1)

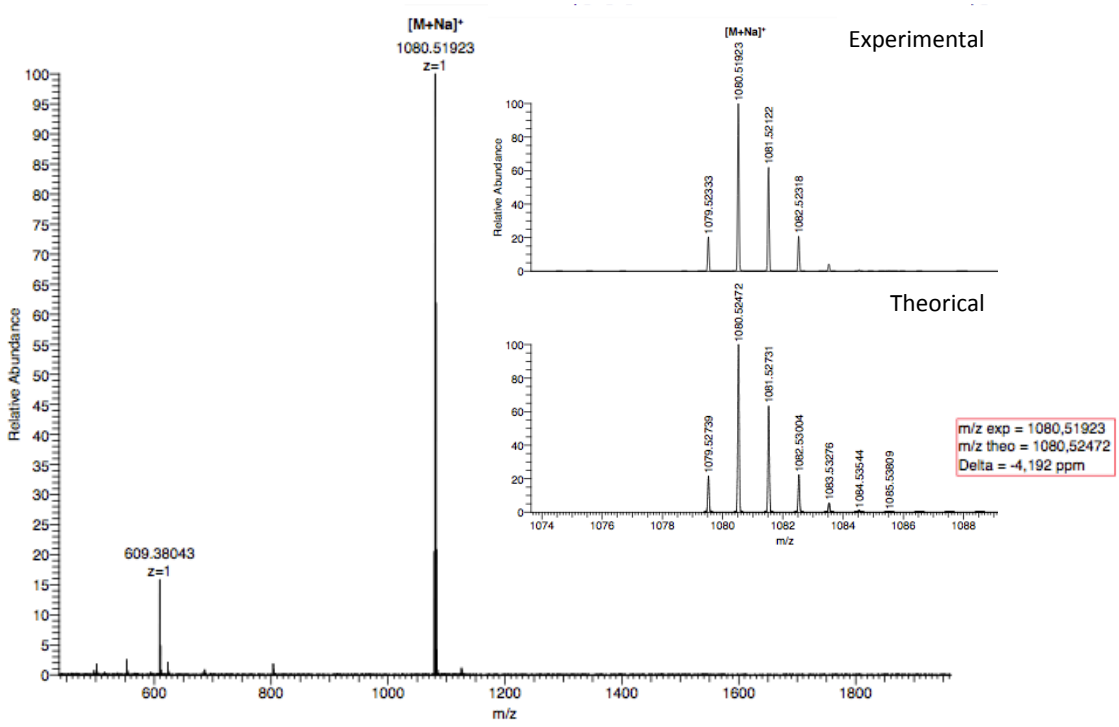

*Fig. S1. HR-MS spectrum of SubPc-DOTAtBu$_3$ (**5**)*

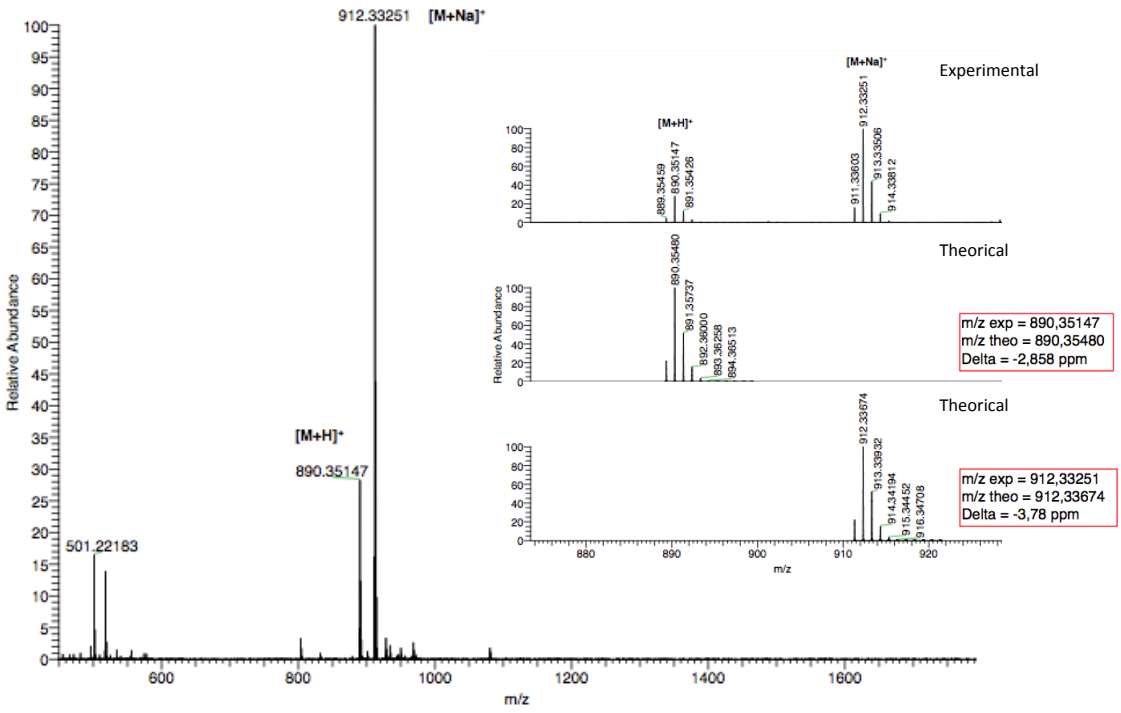

*Fig. S2. HR-MS spectrum of SubPc-DOTA (**1**)*

B.2. SubPc-DTPA (2)

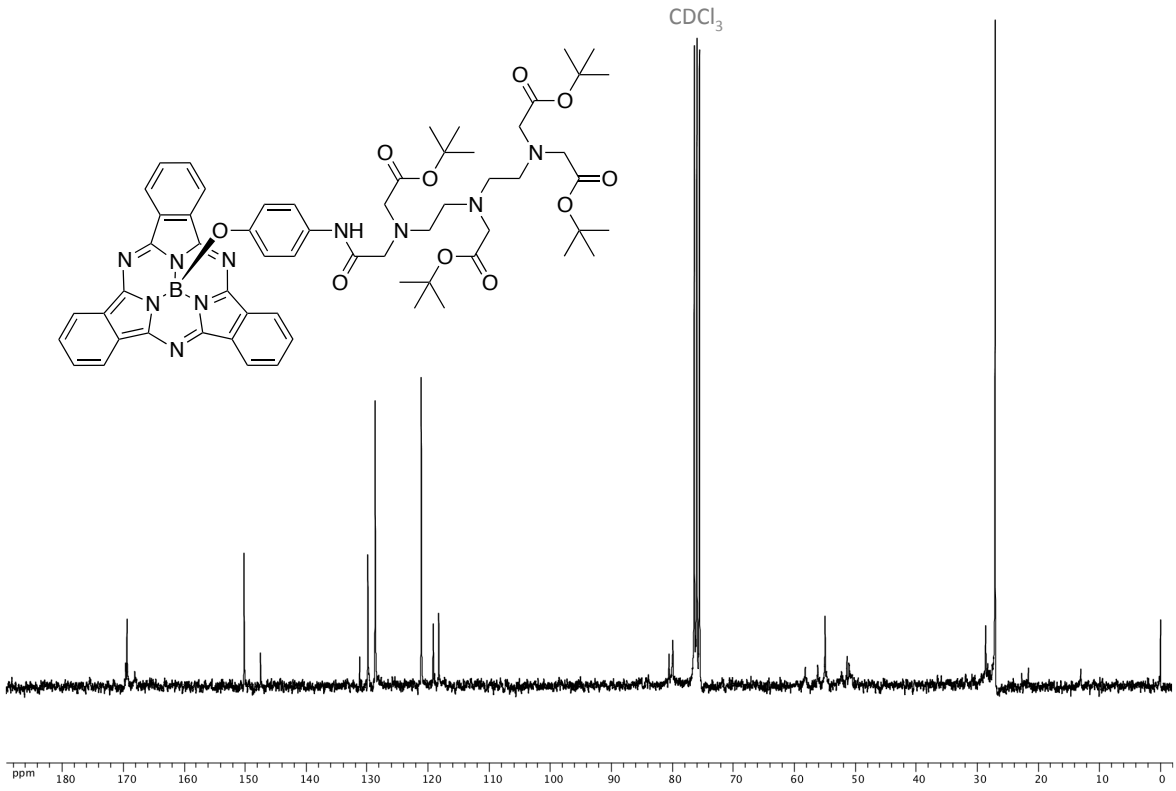

*Fig. S3. ^{13}C NMR spectrum of SubPc-DTPA-tBu$_3$ (**6**) ($CDCl_3$, 75 MHz, 300K)*

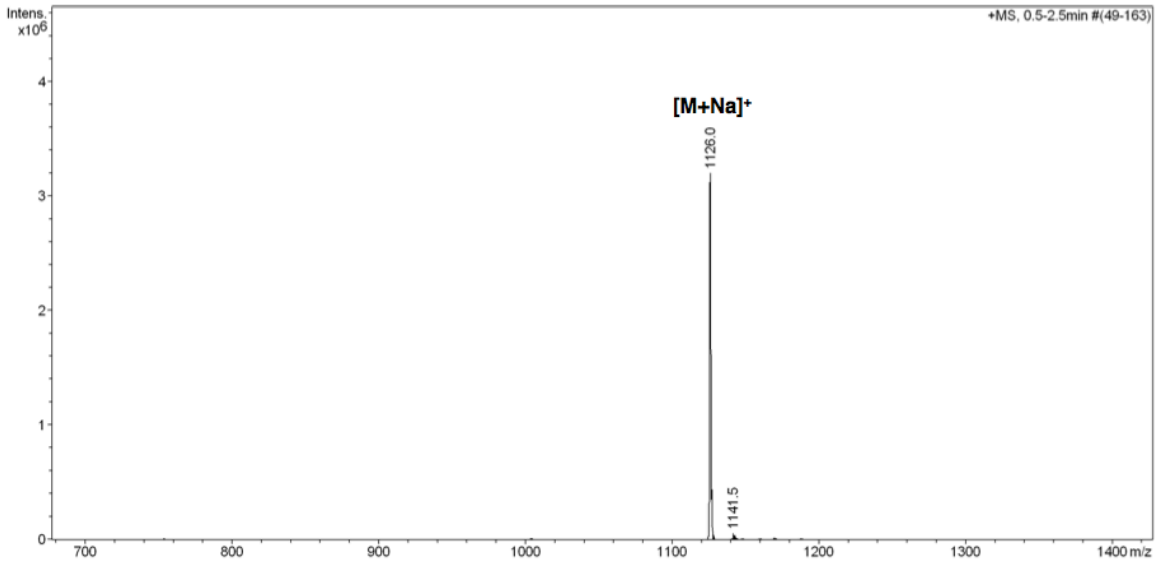

*Fig. S4. MS spectrum of SubPc-DTPA-tBu$_3$ (**6**)*

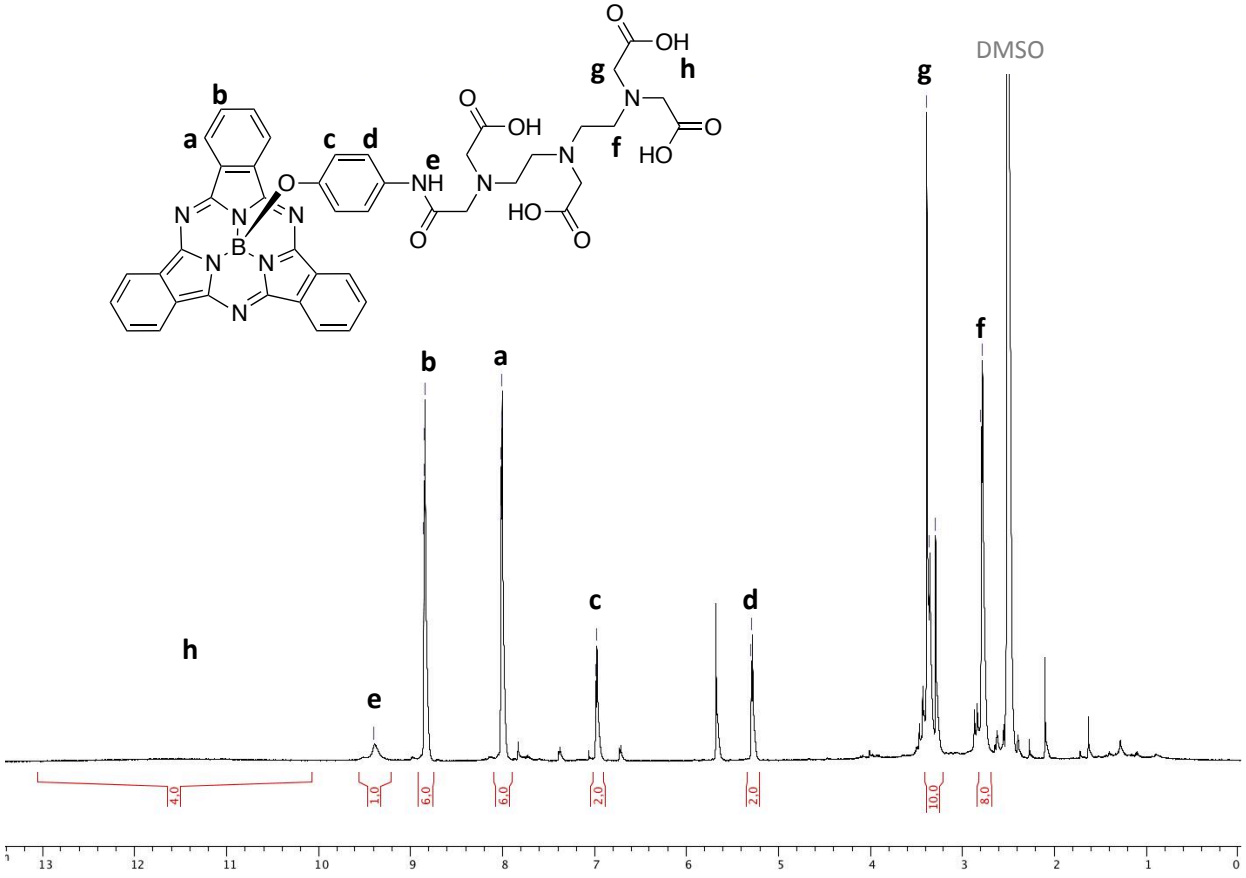

*Fig. S5. ^{1}H NMR spectrum of SubPc-DTPA (**2**) (DMSO, 600 MHz, 400K)*

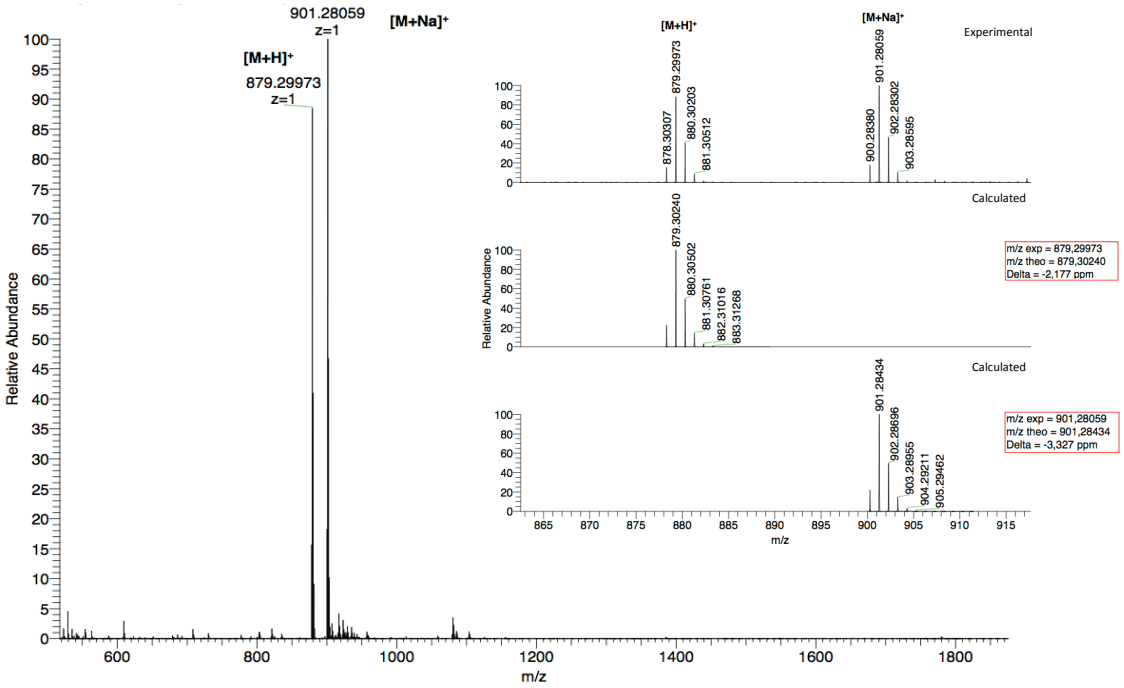

*Fig. S6. HR-MS spectrum of SubPc-DTPA (**2**)*

B.3. SubPc-MDOTA (1-M) and SubPc-MDTPA (2-M)

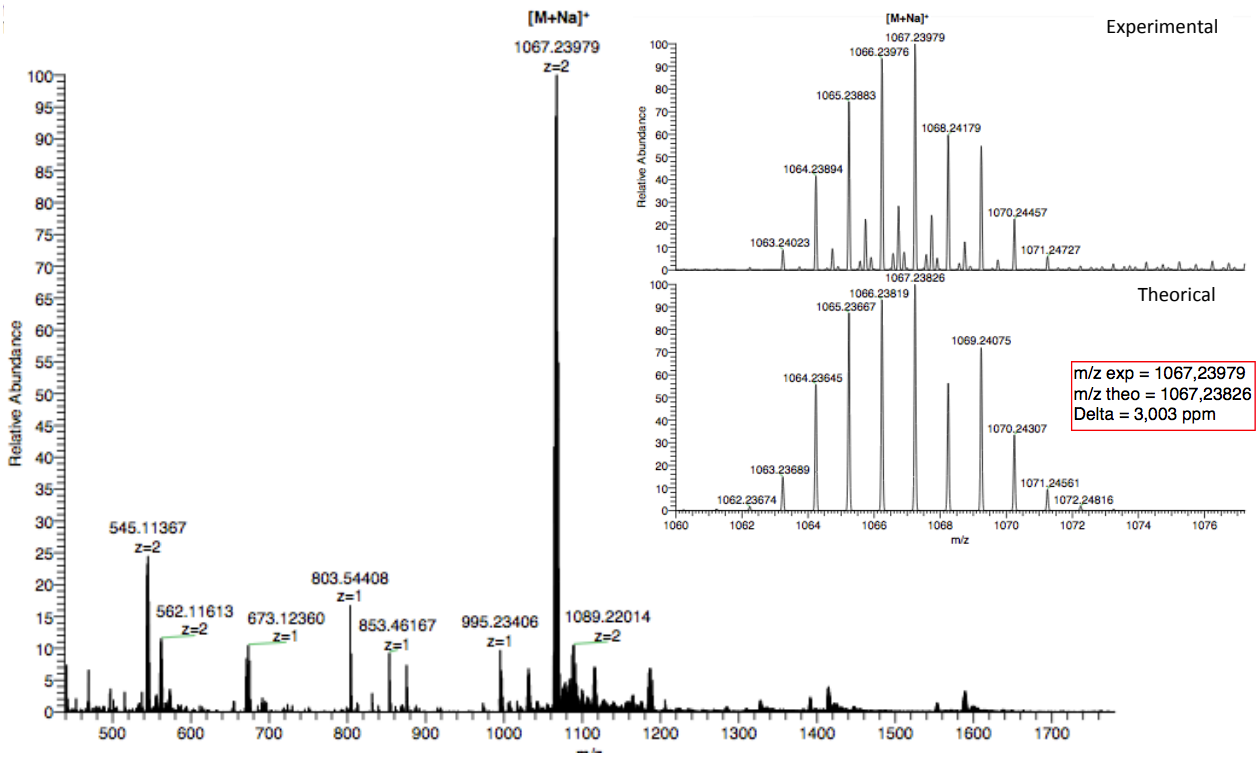

*Fig. S7. HR-MS spectrum of SubPc-GdDOTA (**1-Gd**)*

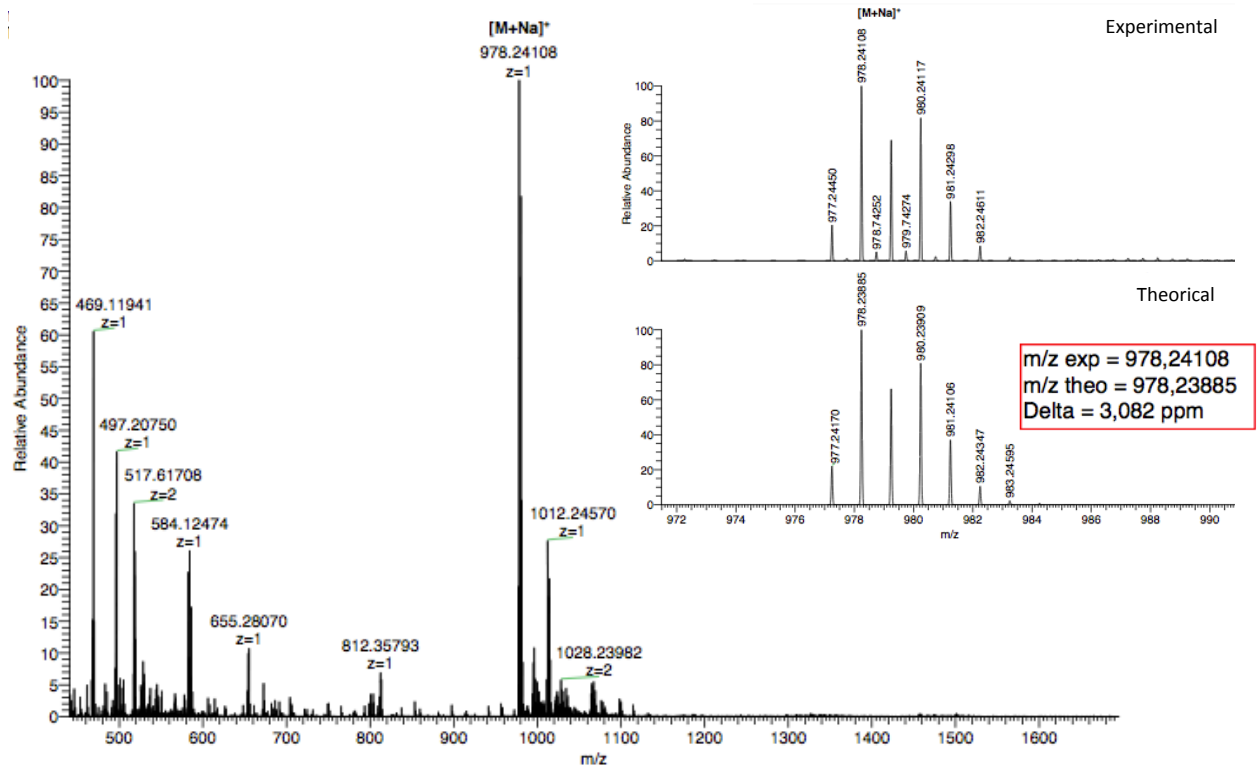

*Fig. S8. HR-MS spectrum of SubPc-GaDOTA (**1-Ga**)*

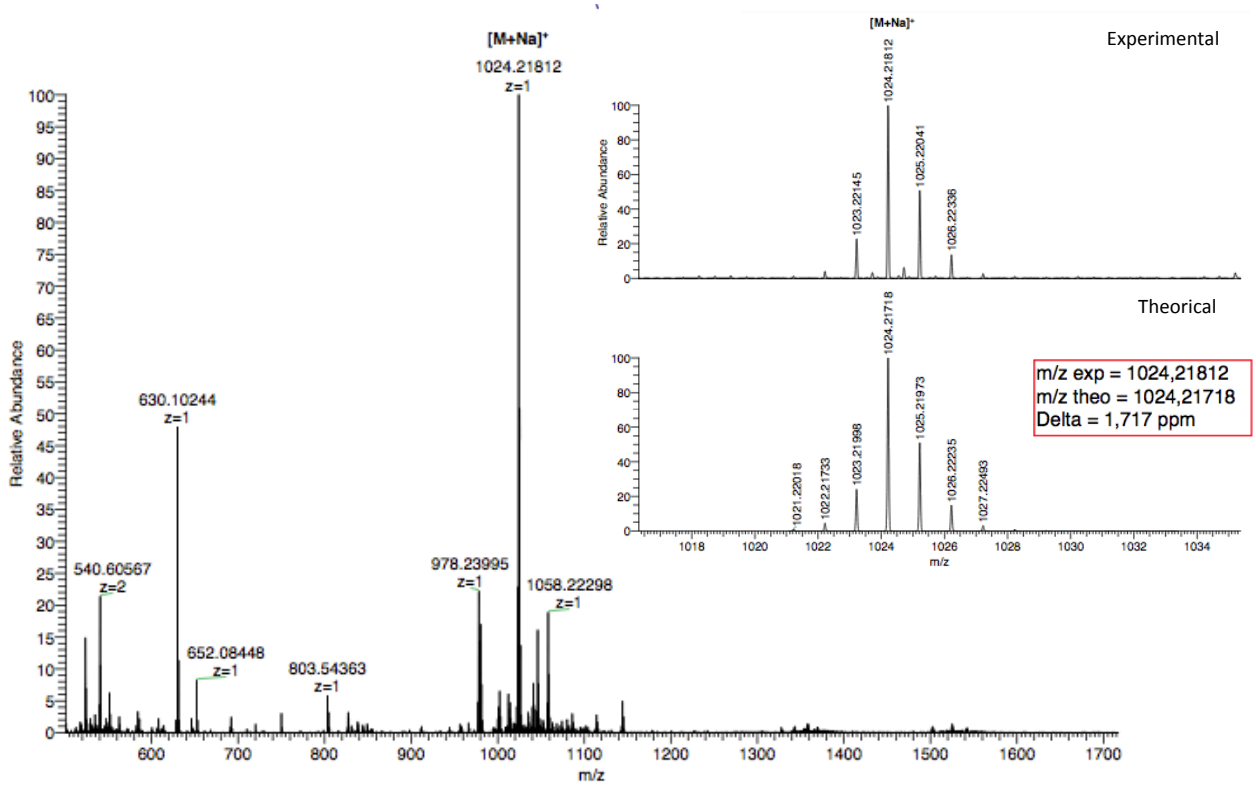

*Fig. S9. HR-MS spectrum of SubPc-InDOTA (**1-In**)*

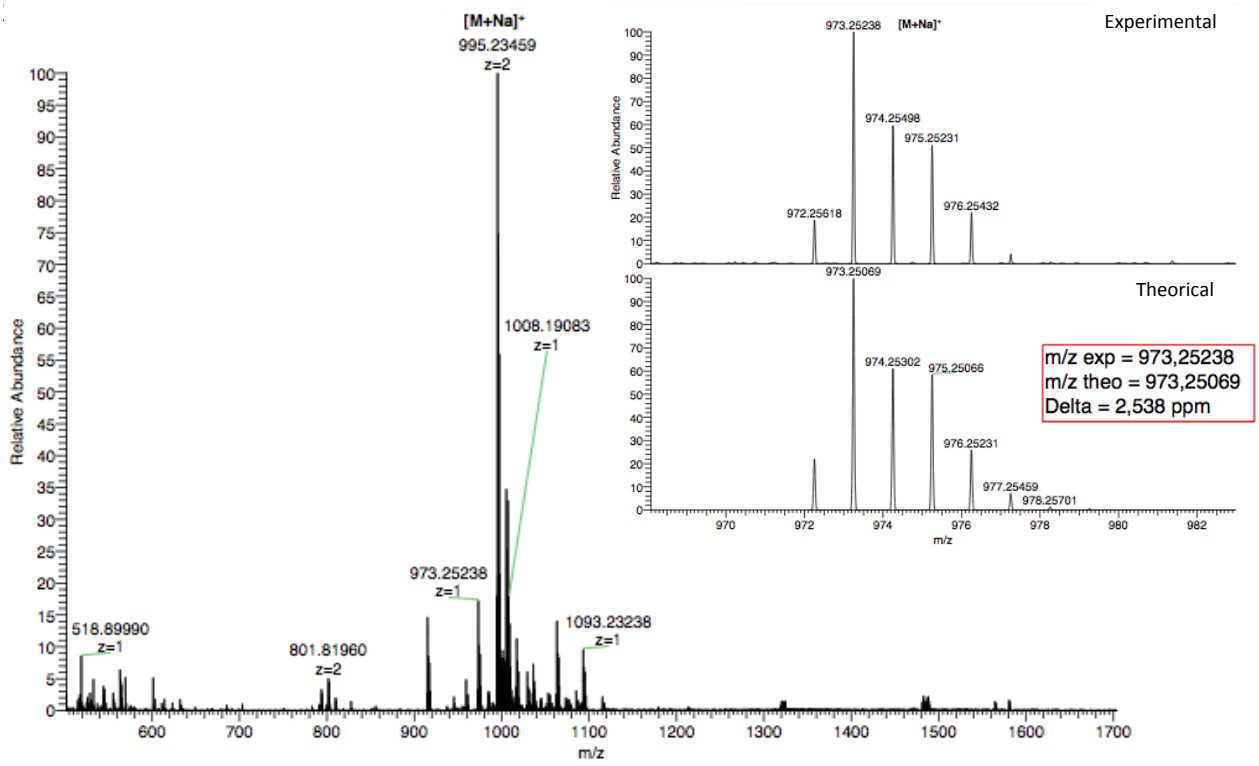

*Fig. S10. HR-MS spectrum of SubPc-LuDOTA (**1-Lu**)*

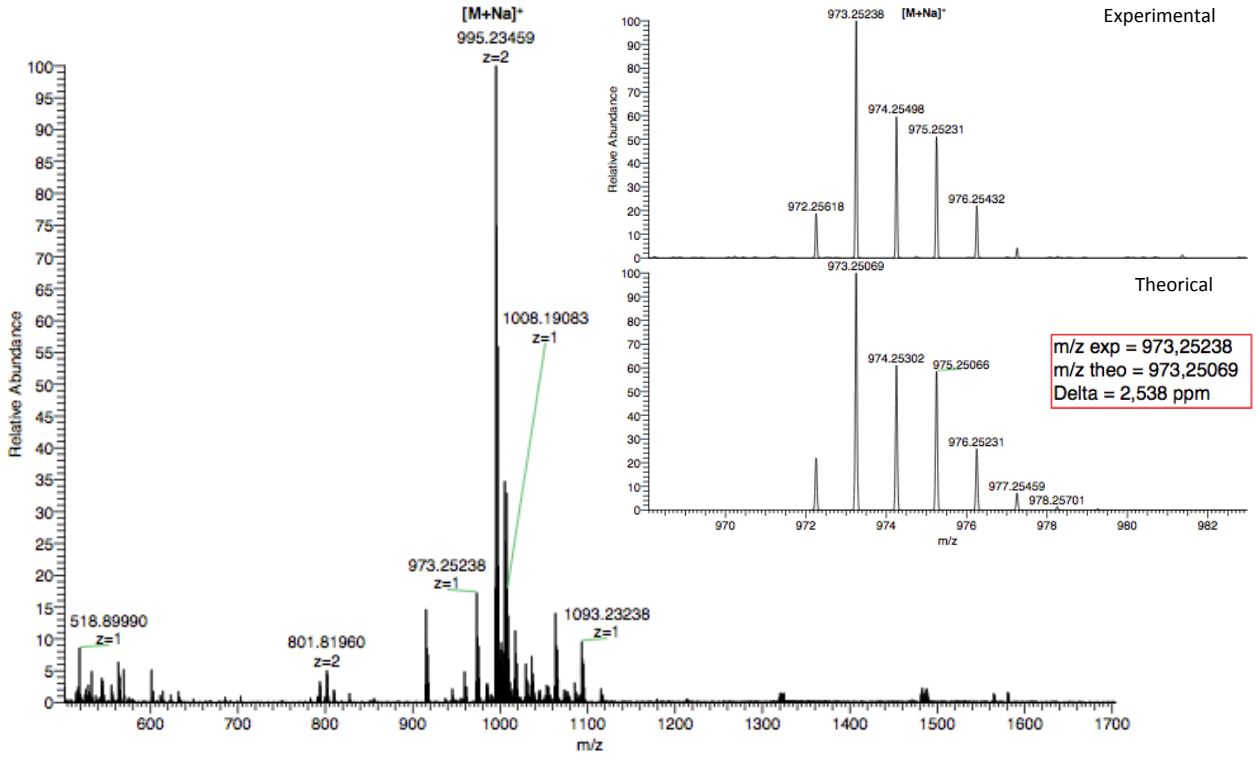

*Fig. S11. HR-MS spectrum of SubPc-LuDOTA (**1-Lu**)*

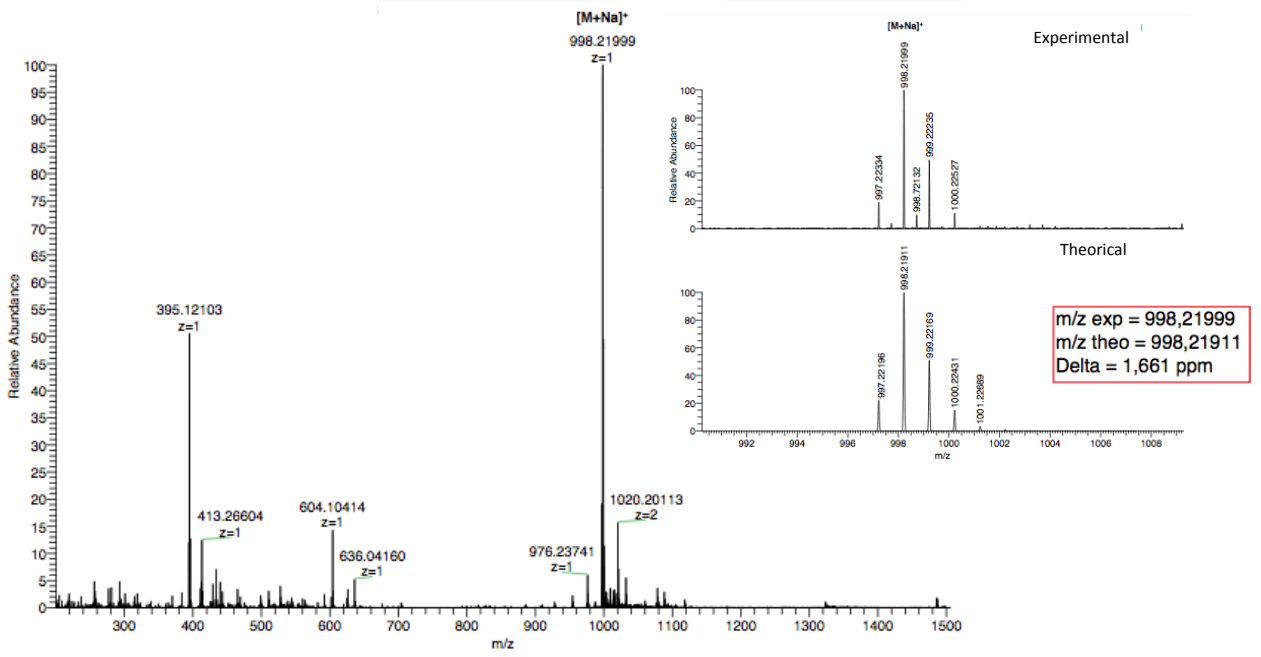

*Fig. S12. HR-MS spectrum of SubPc-LuDOTA (**1-Lu**)*

C. DETECTION OF FREE GADOLINIUM

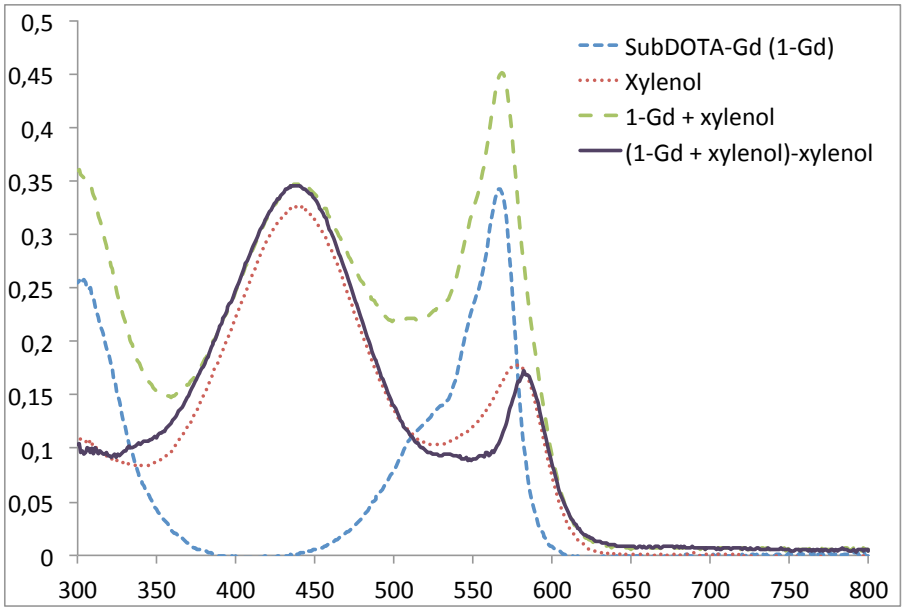

*Fig. S13. Absorption spectra of **1-Gd** in methanol (blue curve), xylenol in water (red curve), mixture of 1-Gd and xylenol (green curve). The full line curve (black curve) correspond to the subtraction of mixture of **1-Gd** and xylenol curve minus the free xylenol curve.*

D. STABILITY STUDIES IN RPMI

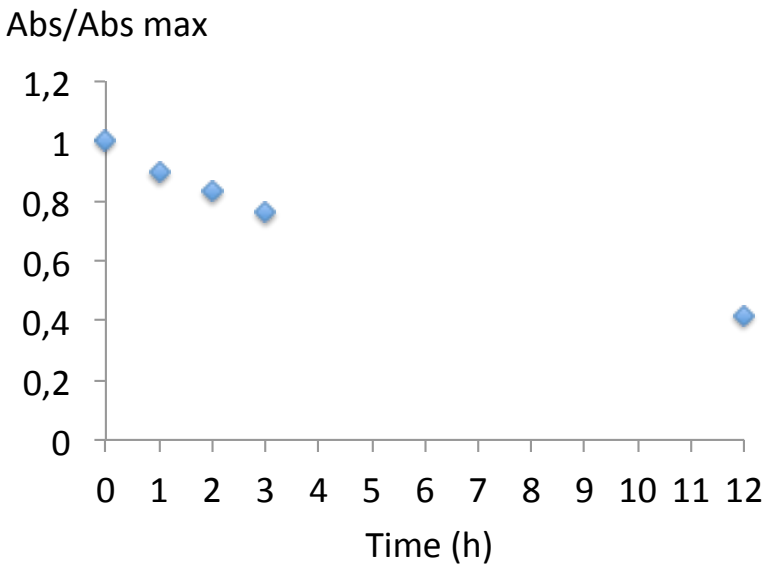

*Fig. S14. Absorption of **1-Gd** in RPMI in dark as a function of time*