

Supporting Information

Design, Synthesis and Biological Evaluation of Choline based SPECT Imaging Agent:

Ga(III)-DO3A-EA-Choline^{†1}

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[†]Electronic supplementary information (ESI) available: Supplementary figures

Figure S1. ^1H NMR spectrum of *N,N*-dimethylaminoethylacetate, **2** [400 MHz; CDCl_3]

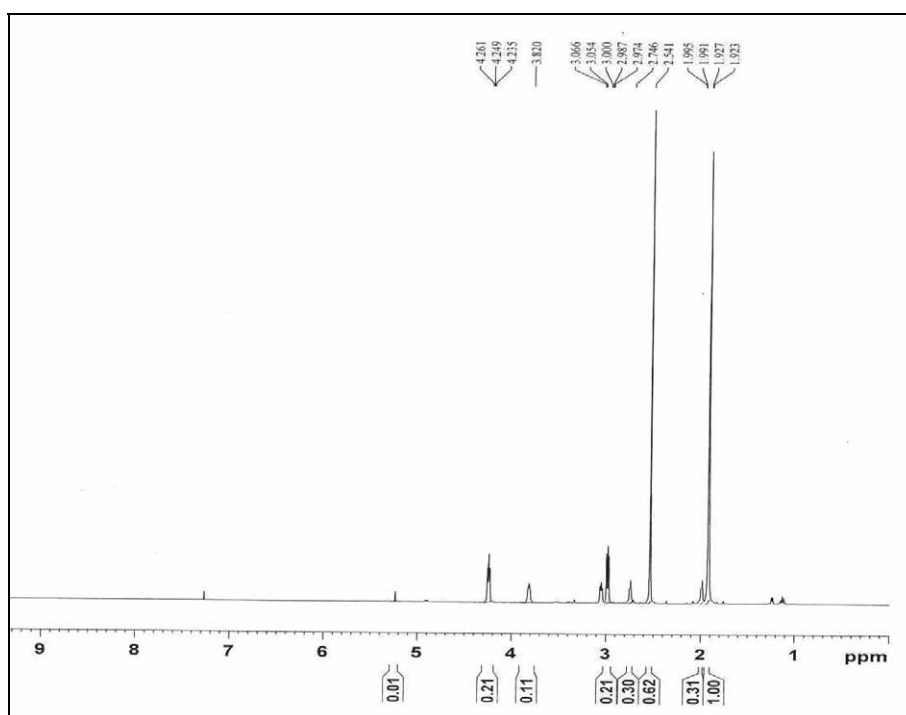


Figure S2. ^{13}C NMR spectrum of *N,N*-dimethylaminoethylacetate, **2** [400 MHz; CDCl_3]

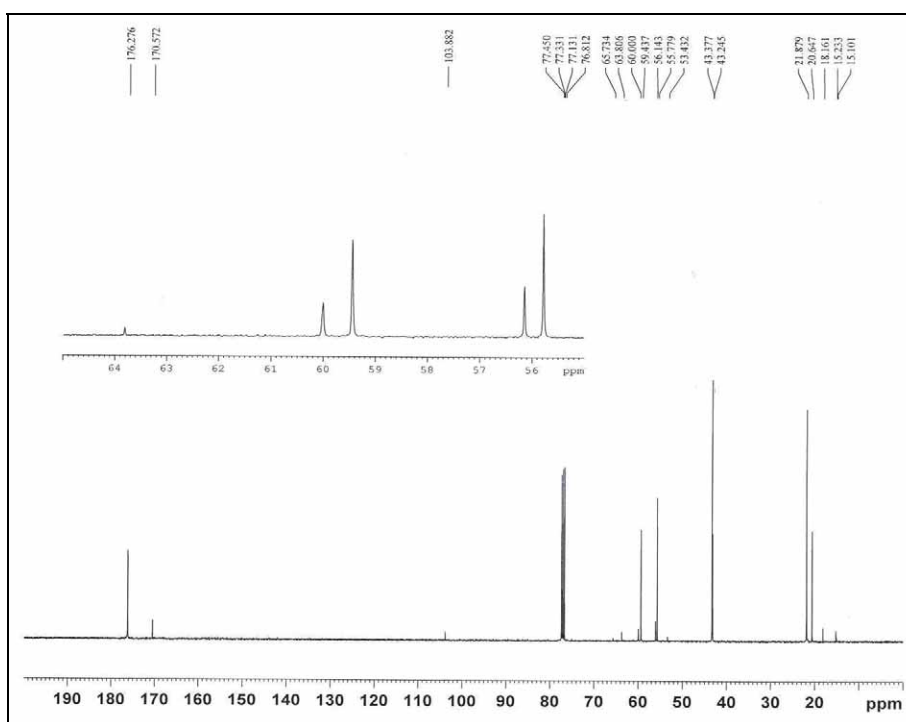


Figure S3. Mass spectrum of *N,N*-dimethylaminoethylacetate, **2** [ESI⁺]

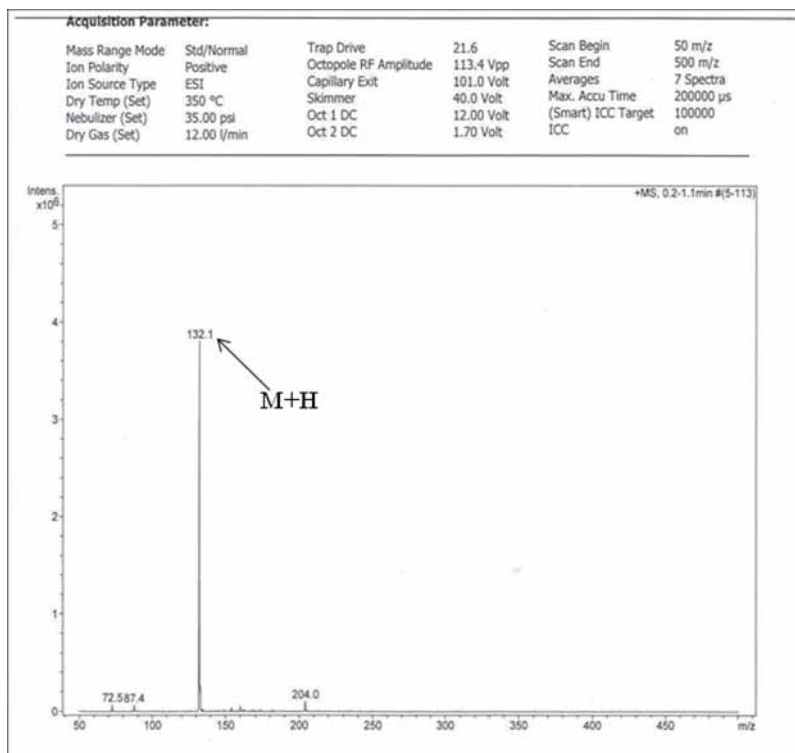


Figure S4. ¹H NMR spectrum of (2-acetoxy-ethyl)-(2-bromo-ethyl)-dimethyl-ammonium, **3** [400 MHz; CDCl₃]

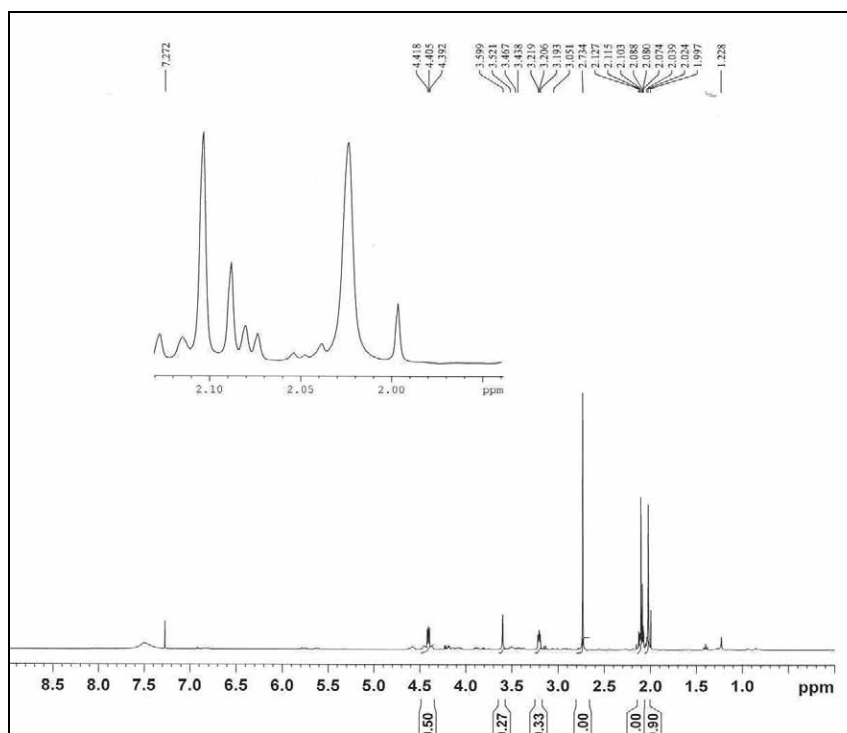


Figure S5. ^{13}C NMR spectrum of (2-acetoxy-ethyl)-(2-bromo-ethyl)-dimethyl-ammonium, **3** [400 MHz; CDCl_3]

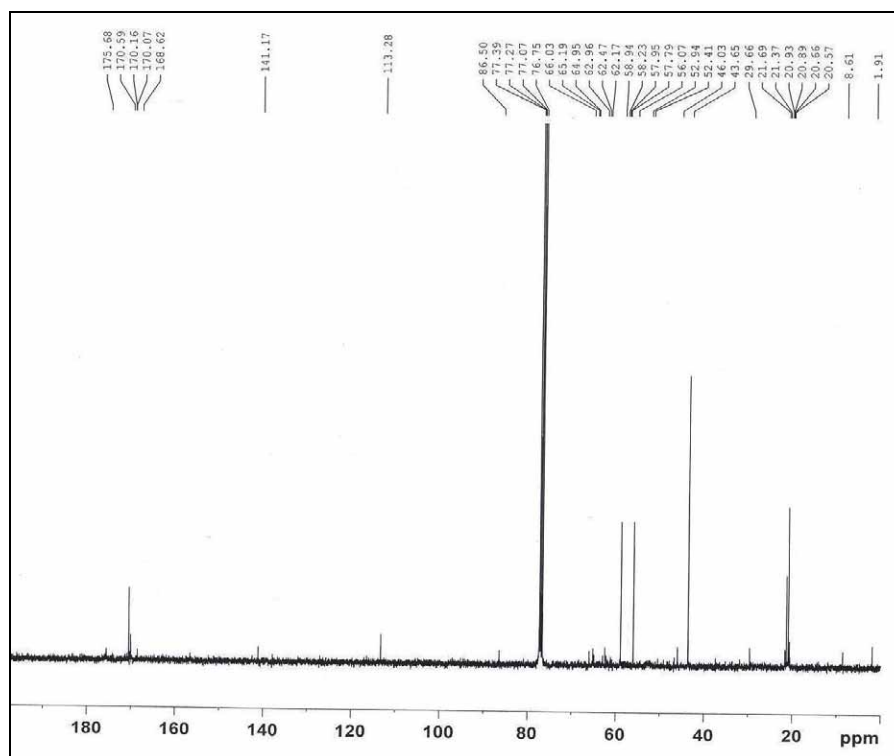


Figure S6. Mass spectrum of (2-acetoxy-ethyl)-(2-bromo-ethyl)-dimethyl-ammonium, **3** [ESI $^+$]

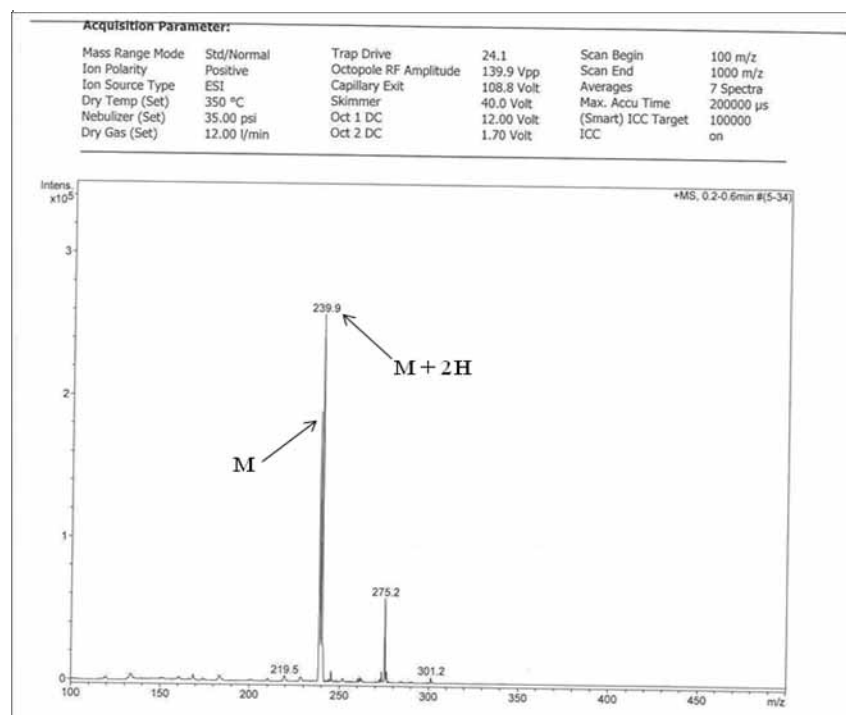


Figure S7. ¹H NMR spectrum of (4,7-bis-*t*-butoxycarbonylmethyl-1,4,7,10 tetraaza-cyclododec-1-yl)-acetic acid *t*-butyl ester, **4** [400 MHz; CDCl₃]

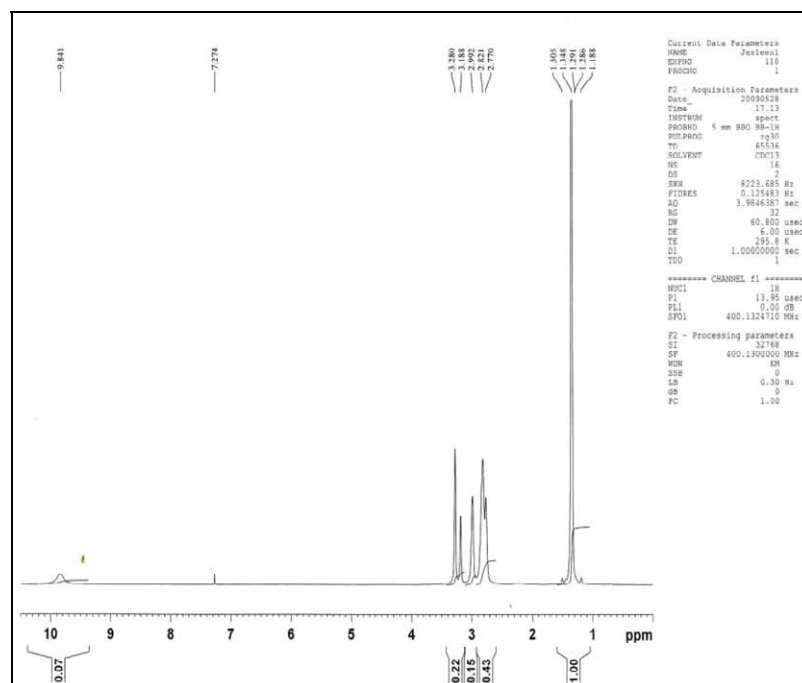


Figure S8. ¹³C NMR spectrum of (4, 7-bis-*t*-butoxycarbonylmethyl-1,4,7,10 tetraaza-cyclododec-1-yl)-acetic acid *t*-butyl ester, **4** [400 MHz; CDCl₃]

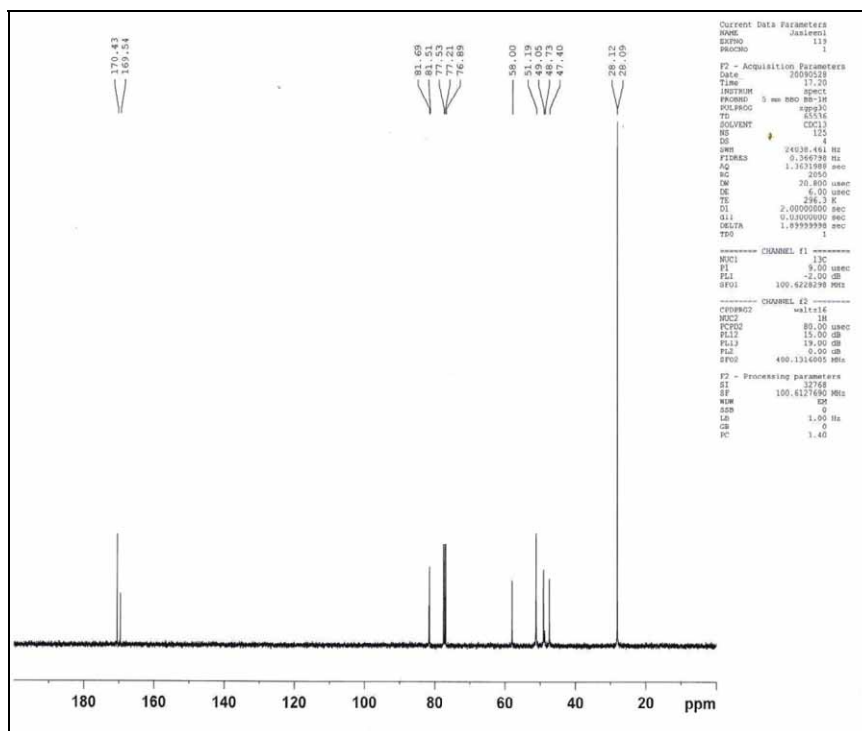
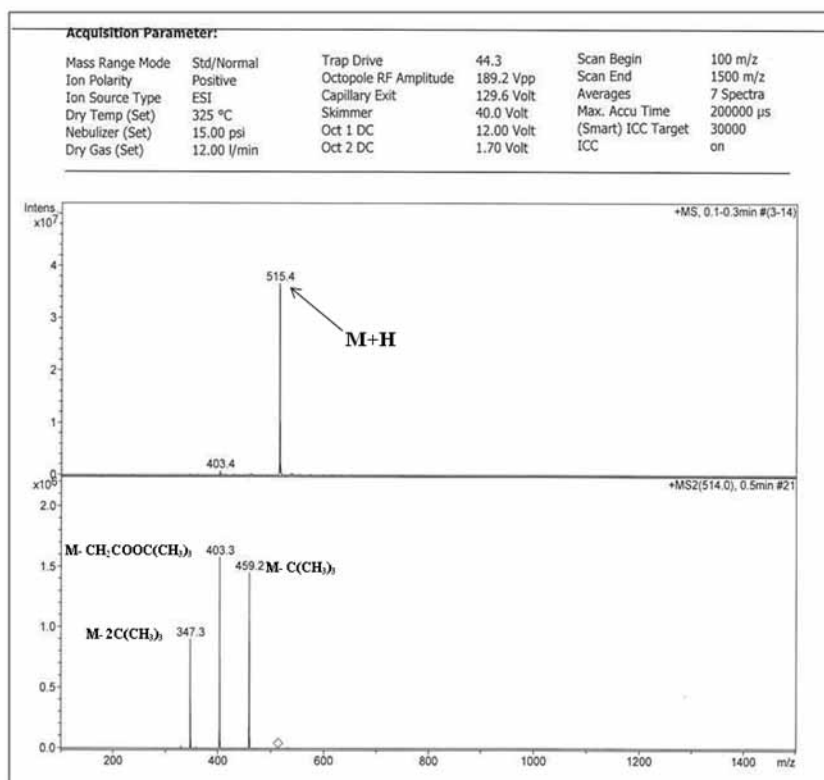


Figure S9. Mass spectrum of (4,7-bis-*t*-butoxycarbonylmethyl-1,4,7,10 tetraaza-cyclododec-1-yl)-acetic acid *t*-butyl ester, **4** [ESI⁺]



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Figure S10. ^1H NMR spectrum of (2-acetoxy-ethyl)-dimethyl-[2-(4,7,10-tris-*tert*-butoxycarbonylmethyl-1,4,7,10-tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **5** [400 MHz; CDCl_3]

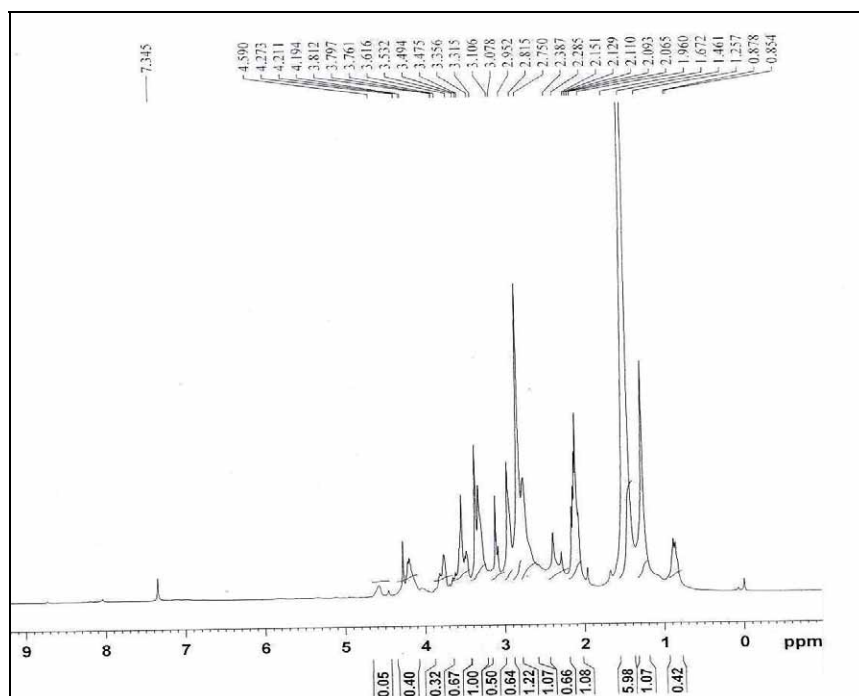


Figure S11. ^{13}C NMR spectrum of (2-acetoxy-ethyl)-dimethyl-[2-(4,7,10-tris-*tert*-butoxycarbonylmethyl-1,4,7,10-tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **5** [400 MHz; CDCl_3]

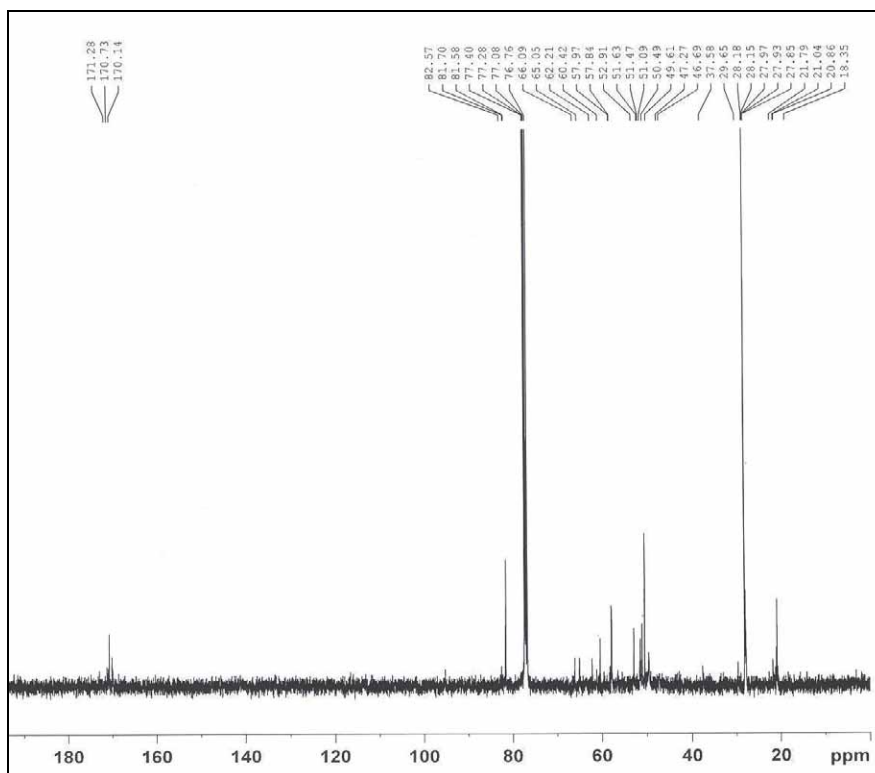


Figure S12. Mass spectrum of (2-acetoxy-ethyl)-dimethyl-[2-(4,7,10-tris-*tert*-butoxycarbonylmethyl-1,4,7,10-tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **5** [ESI⁺]

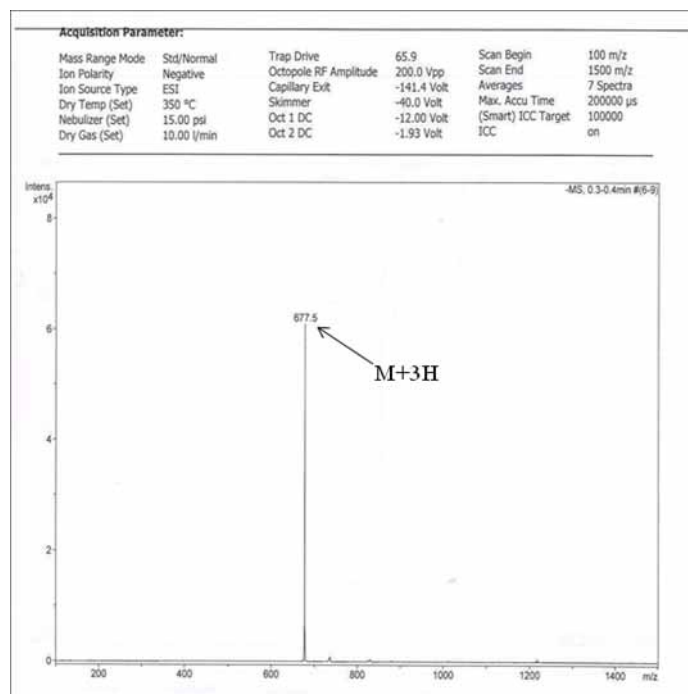


Figure S13. ¹H NMR spectrum of (2-hydroxy-ethyl)-dimethyl-[2-(4,7,10-tris-carboxymethyl-1,4,7,10-tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **6** [400 MHz; D₂O]

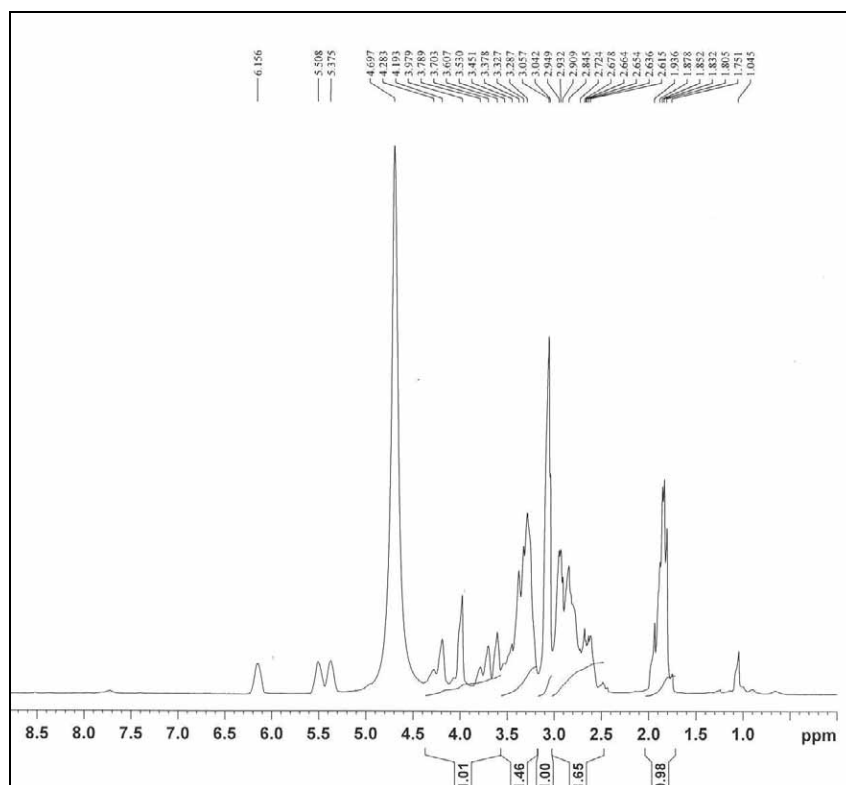


Figure S14. ^{13}C NMR spectrum of (2-hydroxy-ethyl)-dimethyl-[2-(4,7,10-tris-carboxymethyl-1,4,7,10-tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **6** [400 MHz; D_2O]

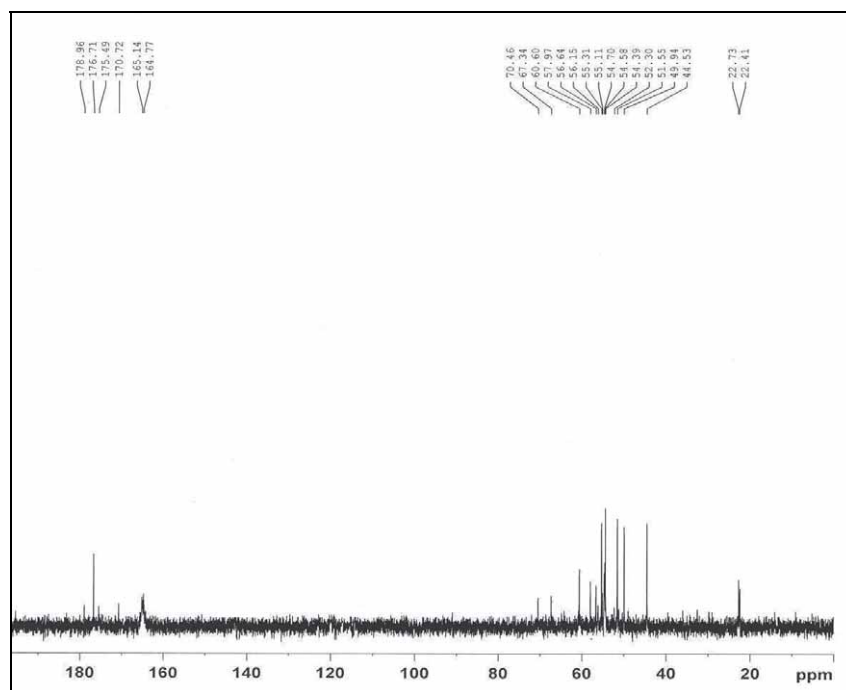


Figure S15. Mass spectrum of (2-hydroxy-ethyl)-dimethyl-[2-(4,7,10-tris-carboxymethyl-1,4,7,10 tetraaza-cyclododec-1-yl)-ethyl]-ammonium, **6** [ESI^+]

