

Supporting Information

Synthesis of Carborane-Containing Cholesterol Derivative and Evaluation as Potential Dual Agent for MRI-BNCT Applications

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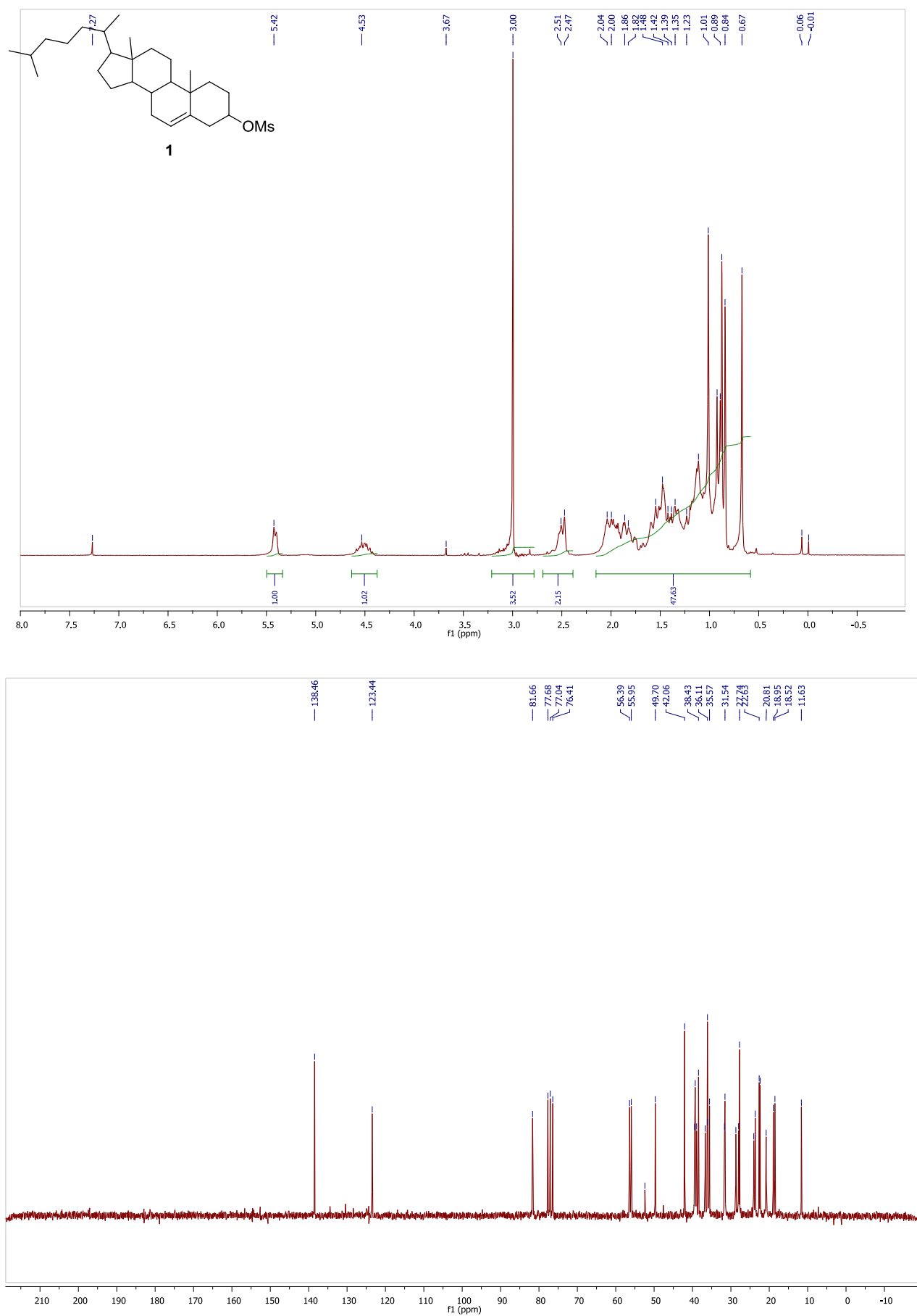
Figure 1 ^1H , ^{13}C of (3 β)-colest-5-en-3-methanesulfonate (**1**)

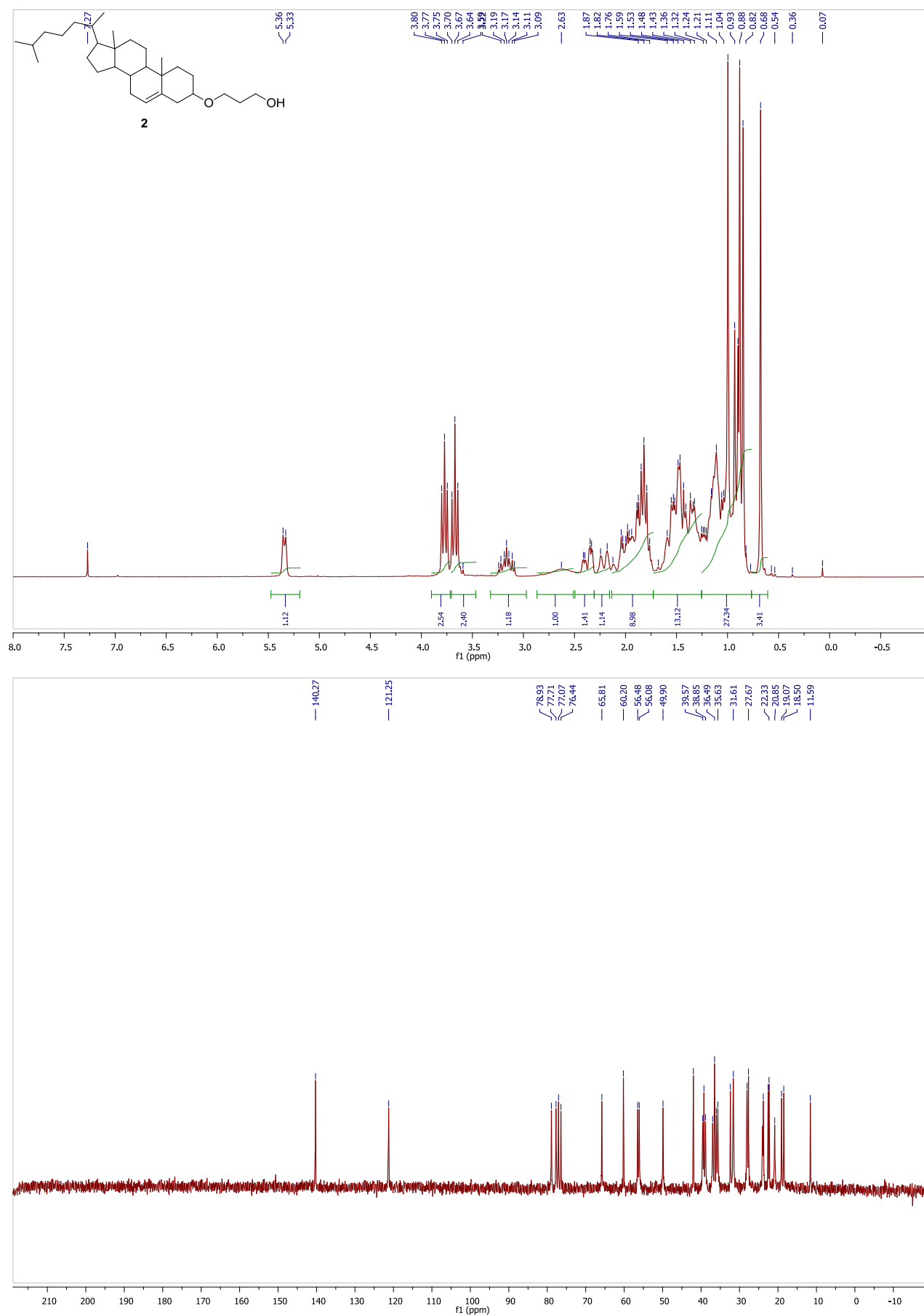
Figure 2 ^1H , ^{13}C of 3-((3 β)-colest-5-en-3-yloxy)-propanol (**2**)

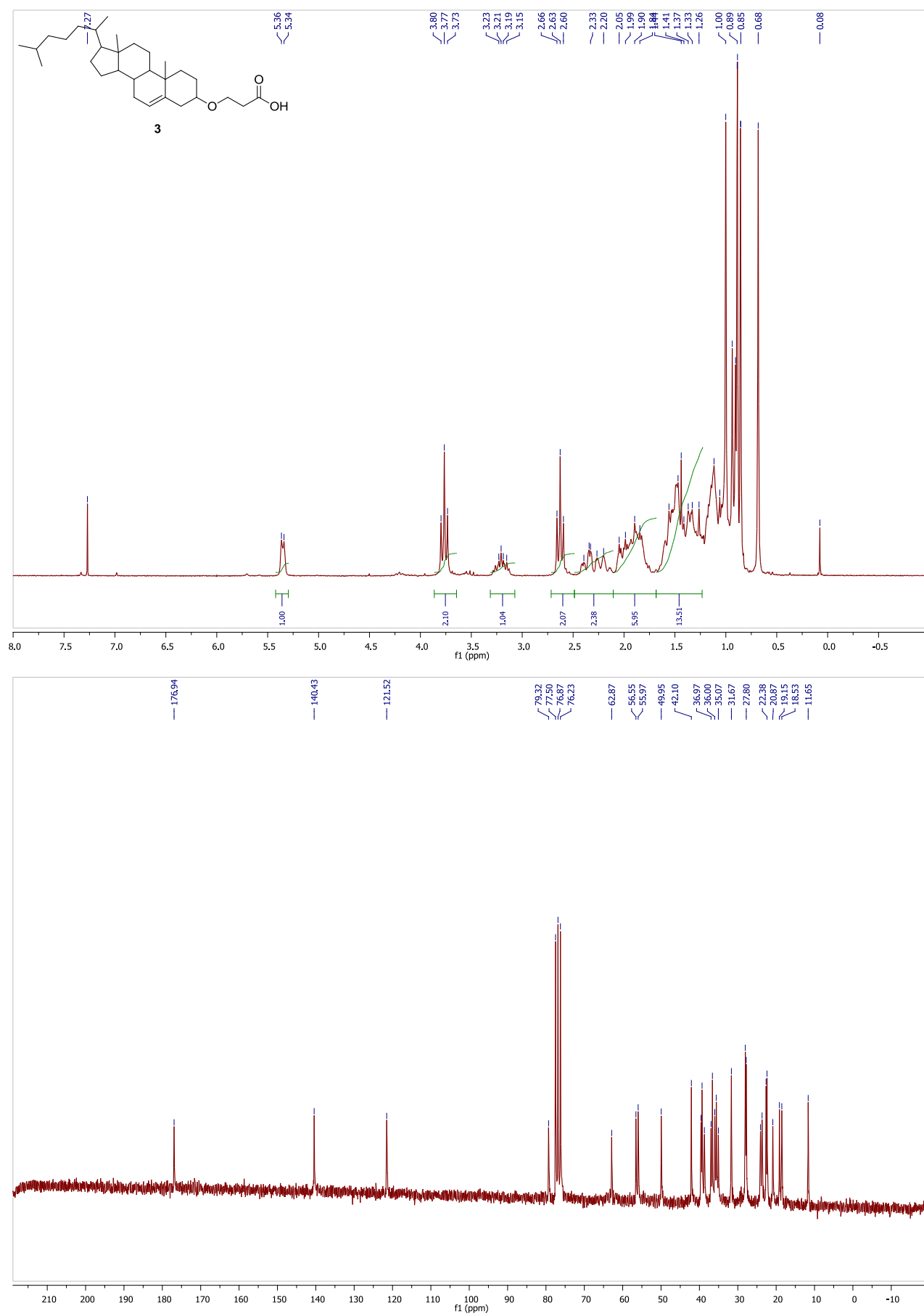
Figure 3 ^1H , ^{13}C of 3-(Cholesten-5-en-3 β -yloxy)-propionic acid (**3**)

Figure 4 ^1H , ^{13}C of C-(2-Benzoyloxyethyl)-C'-[cholesten-5-en-3 β -yloxy-(3-propionacetoamidomethyl)]-o-carborane (**4**)

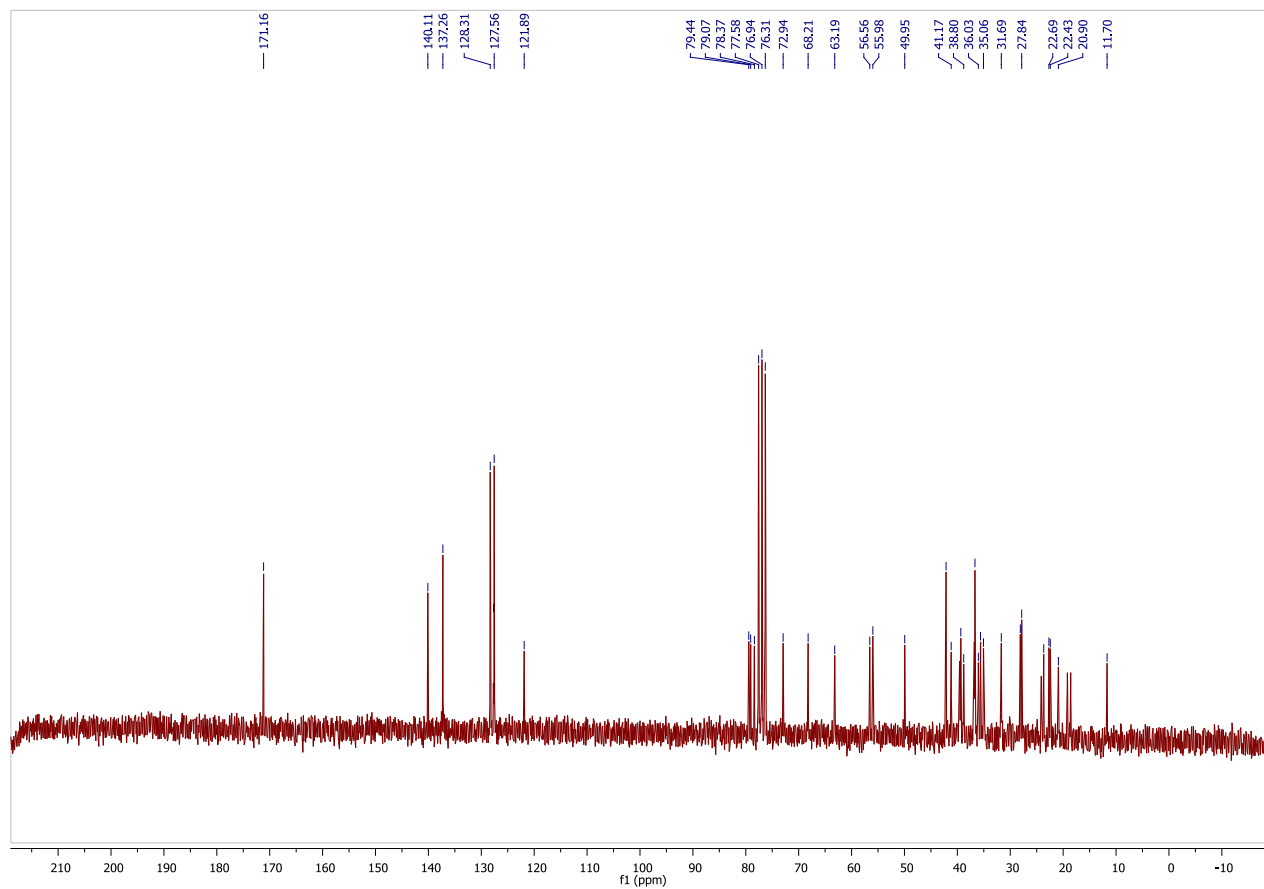
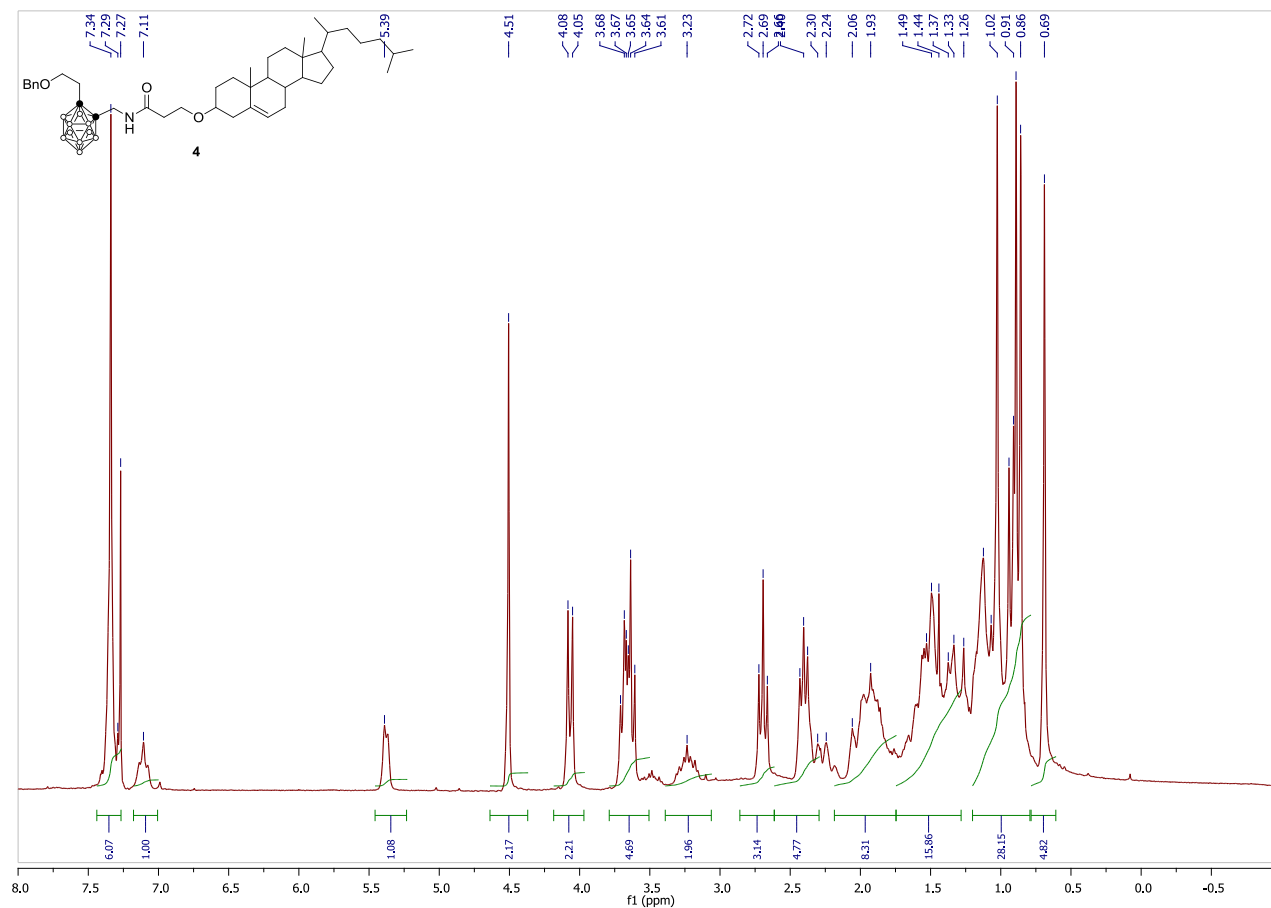


Figure 5 ^1H , ^{13}C of C-(Hydroxyethyl)-C'-[cholesten-5-en-3 β -yloxy-(3-propionacetoamidomethyl)]-o-carborane (**5**)

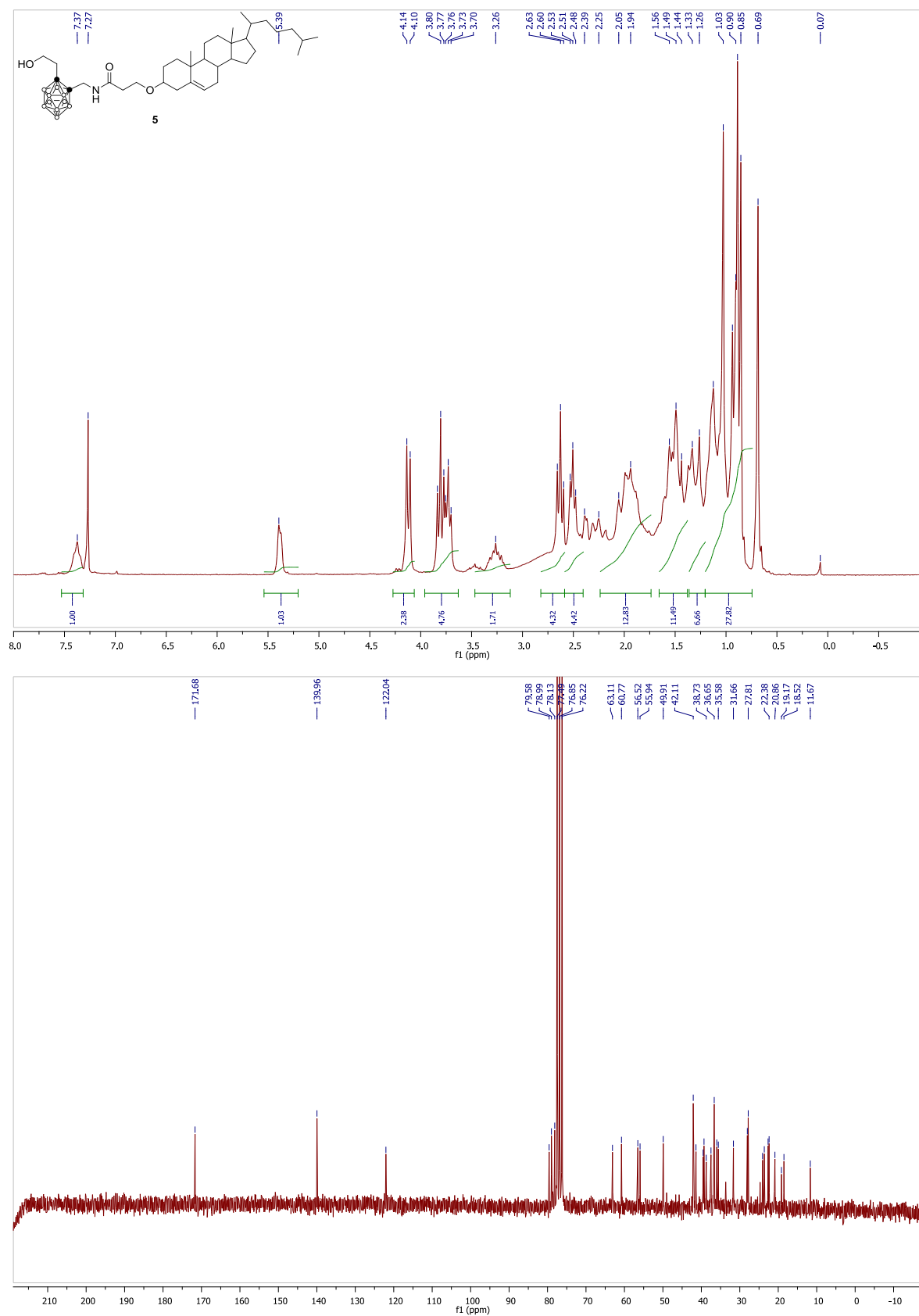


Figure 6 ^1H , ^{13}C of C-[N-*tert*-ButylDOTAMA- C_6]-carbamoylmethyl]-C'-[cholesten-5-en-3 β -yloxy-(3-propionacetoamidomethyl)-*o*-carborane (**8**)

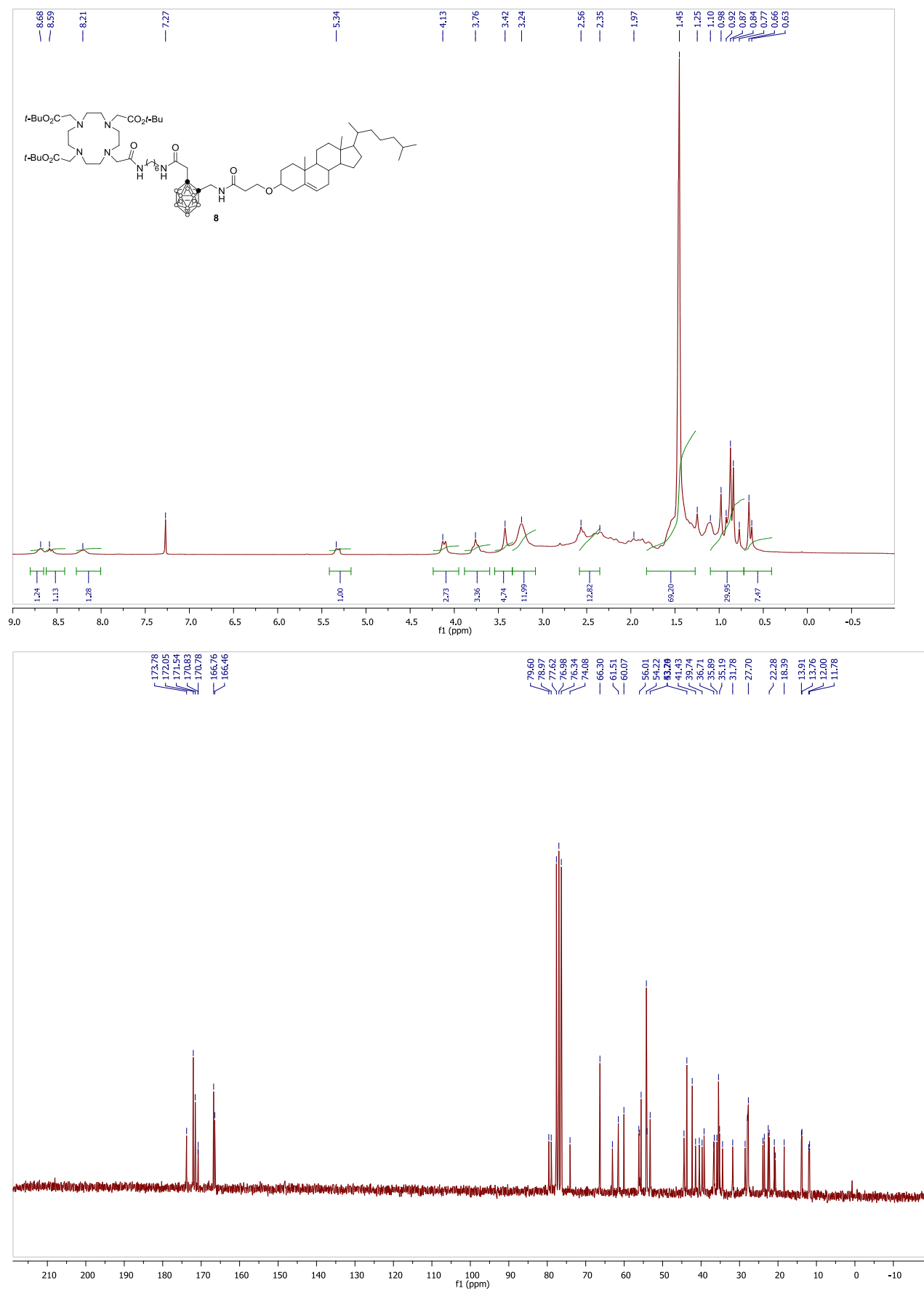


Figure 7 ESI mass spectra of C-[DOTAMA-C₆]-carbamoylmethyl]-C'-[cholesten-5-en-3 β -yloxy-(3-propionacetoamidomethyl)-*o*-carborane (**9**)

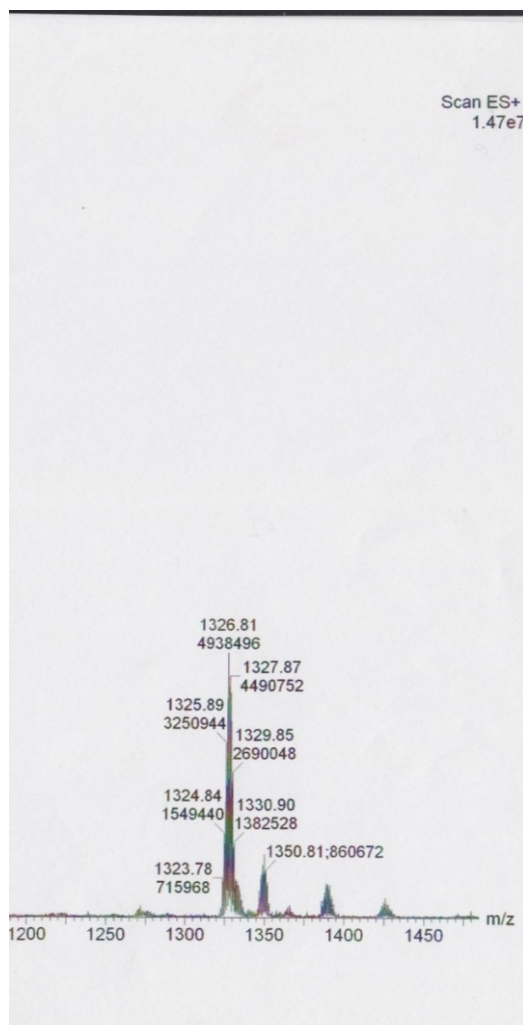
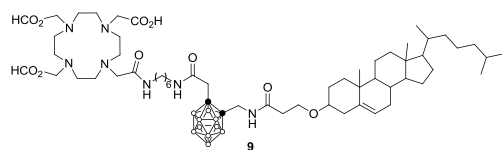


Figure 8 ^1H , ^{13}C spectrum of *C*-(2-benzyloxyethyl)-*C'*-aminomethyl-*o*-carborane (**7**)