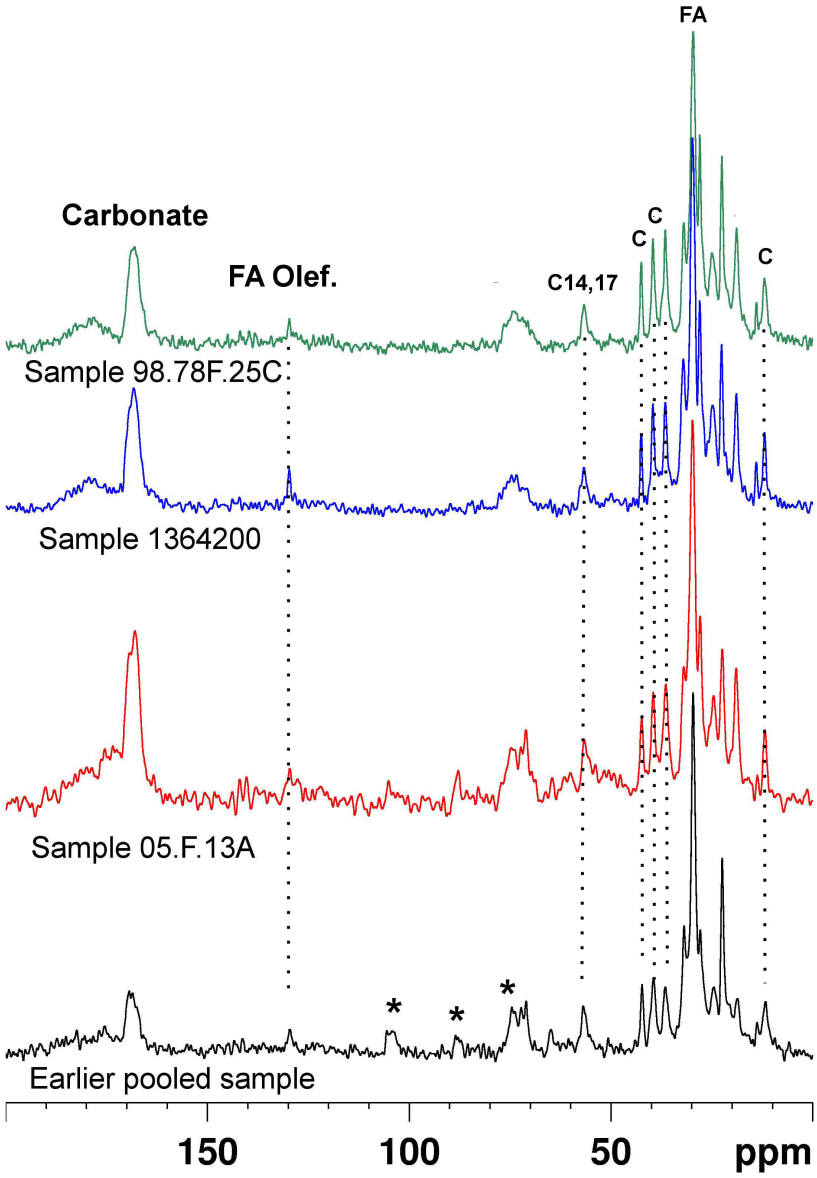
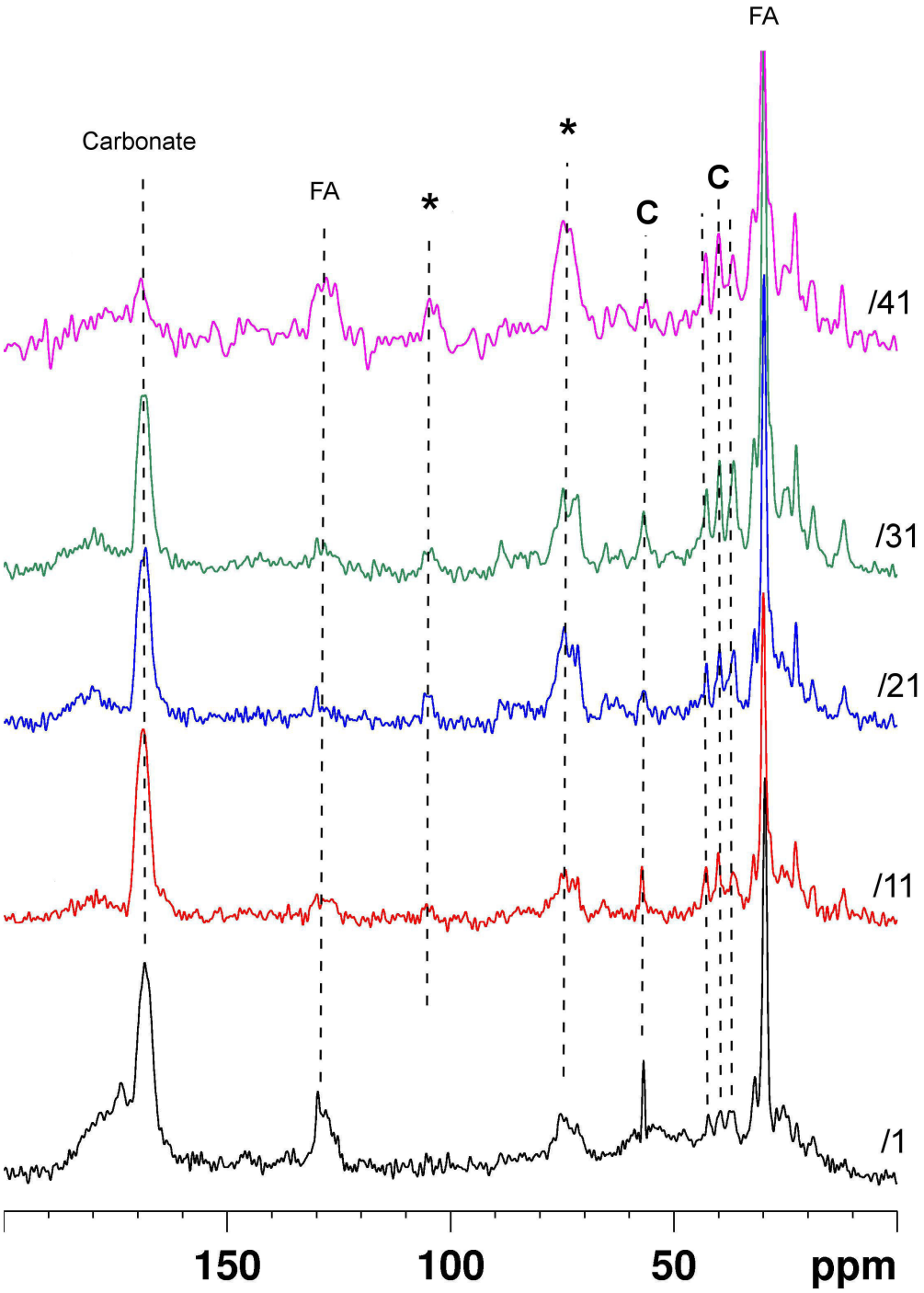
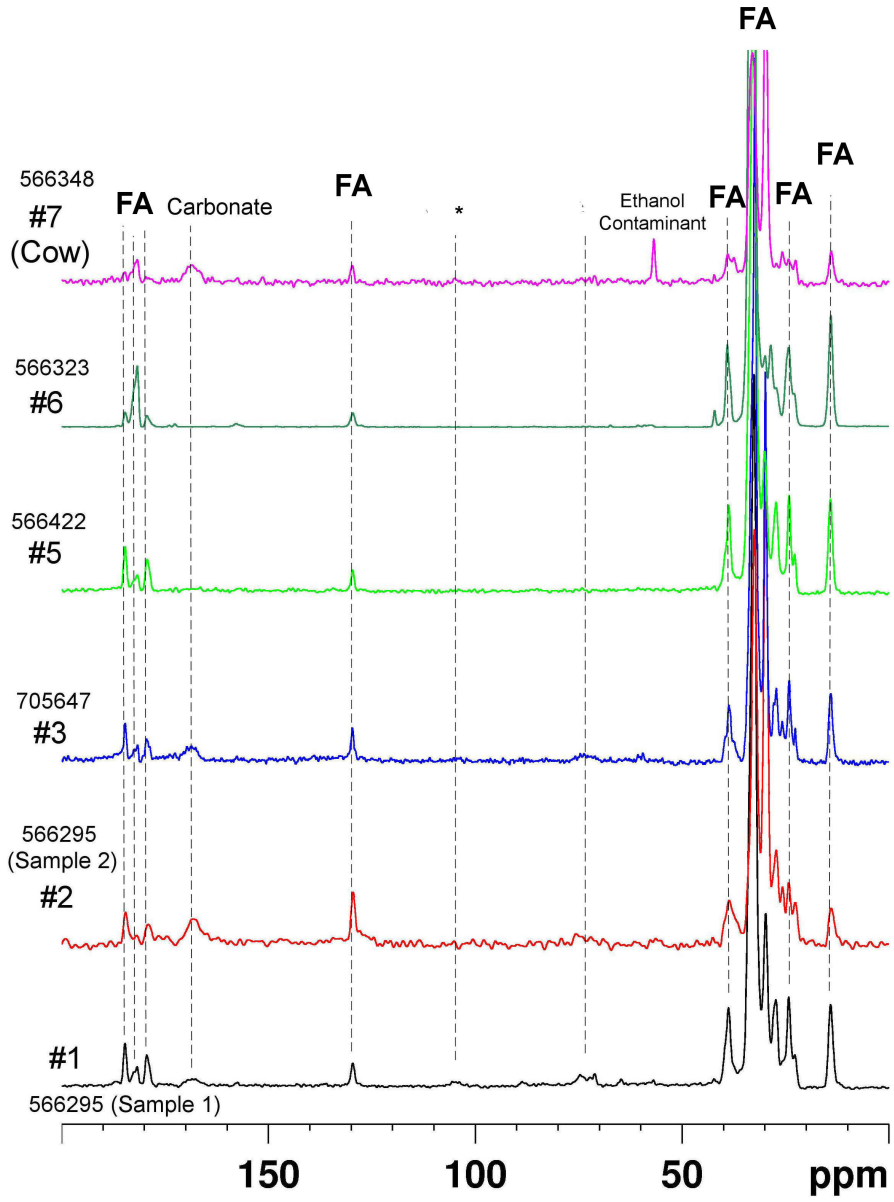
SUPPLEMENTAL



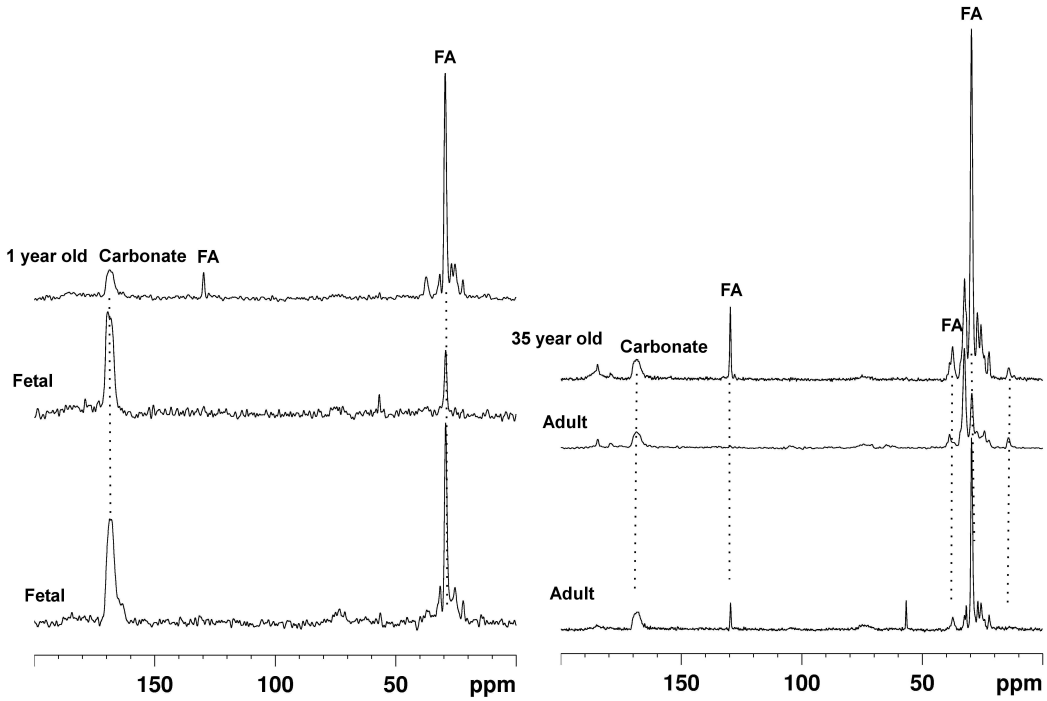
Supplemental I ^{13}C solid state NMR spectra of four samples of mineral from human carotid artery intimal atherosclerotic plaque calcifications. One sample was purified from pooled material from three earlier samples. Abbreviations and symbols have the same meaning as defined in the caption to Figure 1.



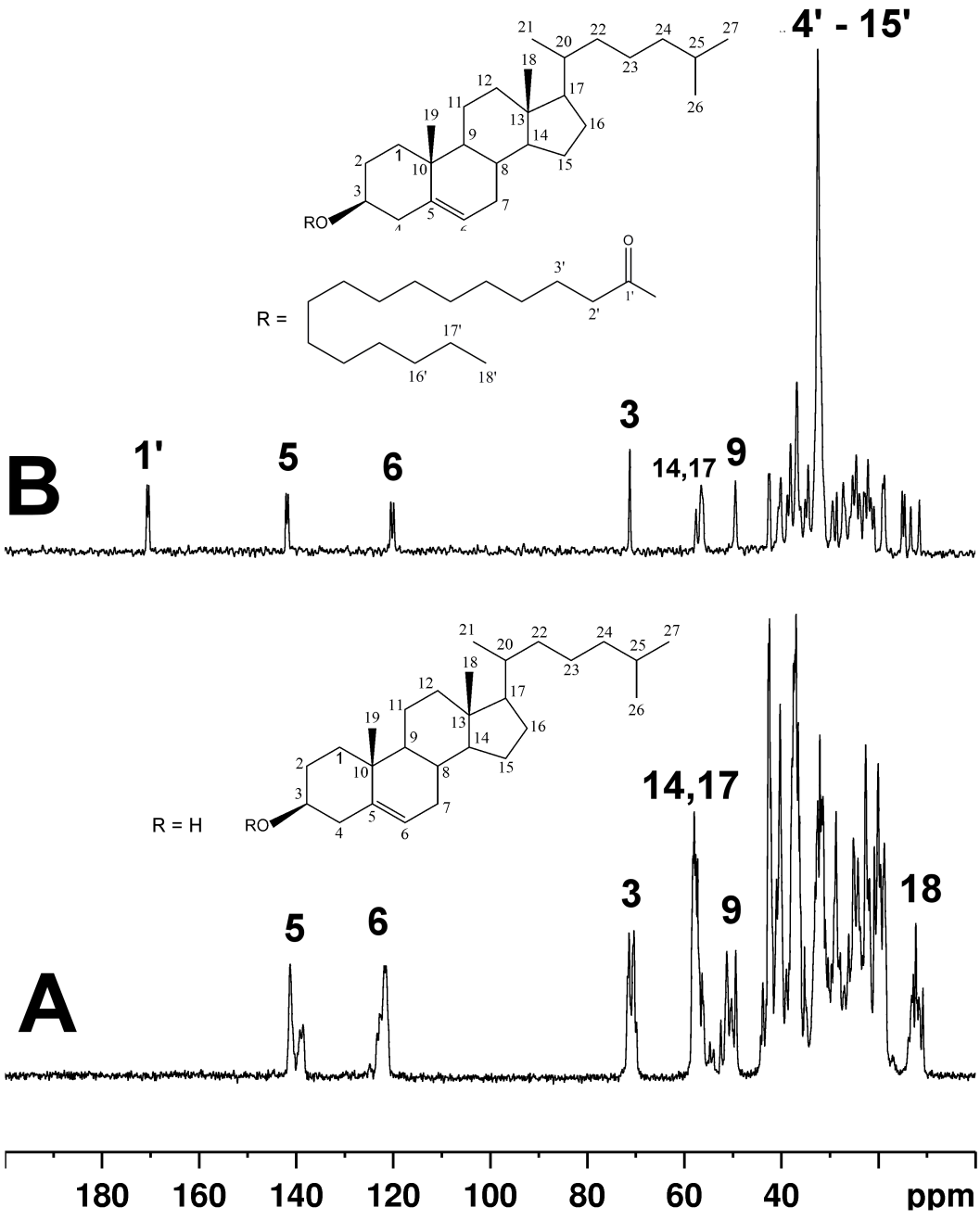
Supplemental II ^{13}C solid state NMR spectra of five samples of mineral from human medial plaque calcifications, all containing an unknown proportion of intimal calcification. Asterisks mark cellulose from filter paper.



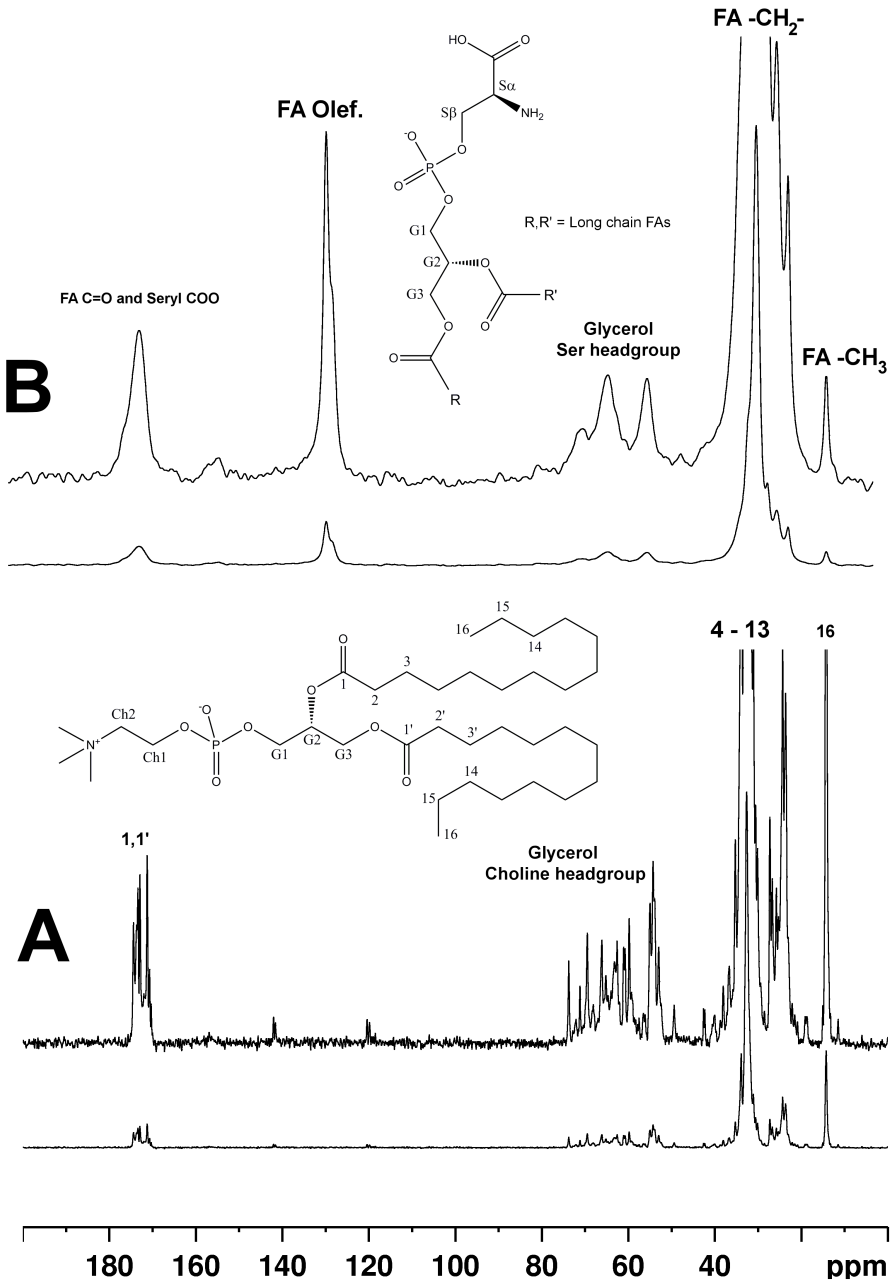
Supplemental III ^{13}C solid state NMR spectra of five samples of equine and one sample of bovine medial vascular calcifications.



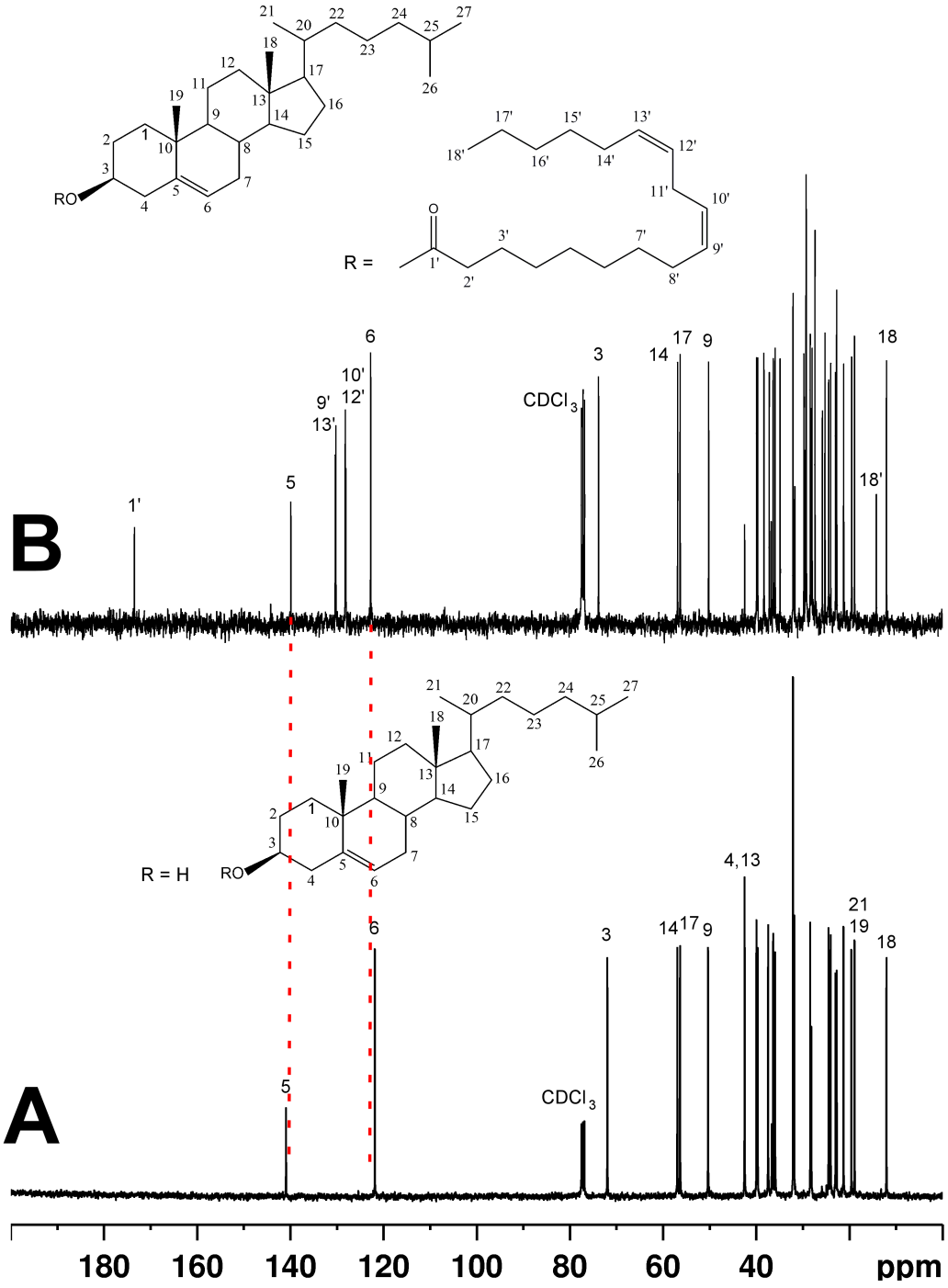
Supplemental IV ^{13}C solid state NMR spectra of six samples of equine bone mineral from different donors.



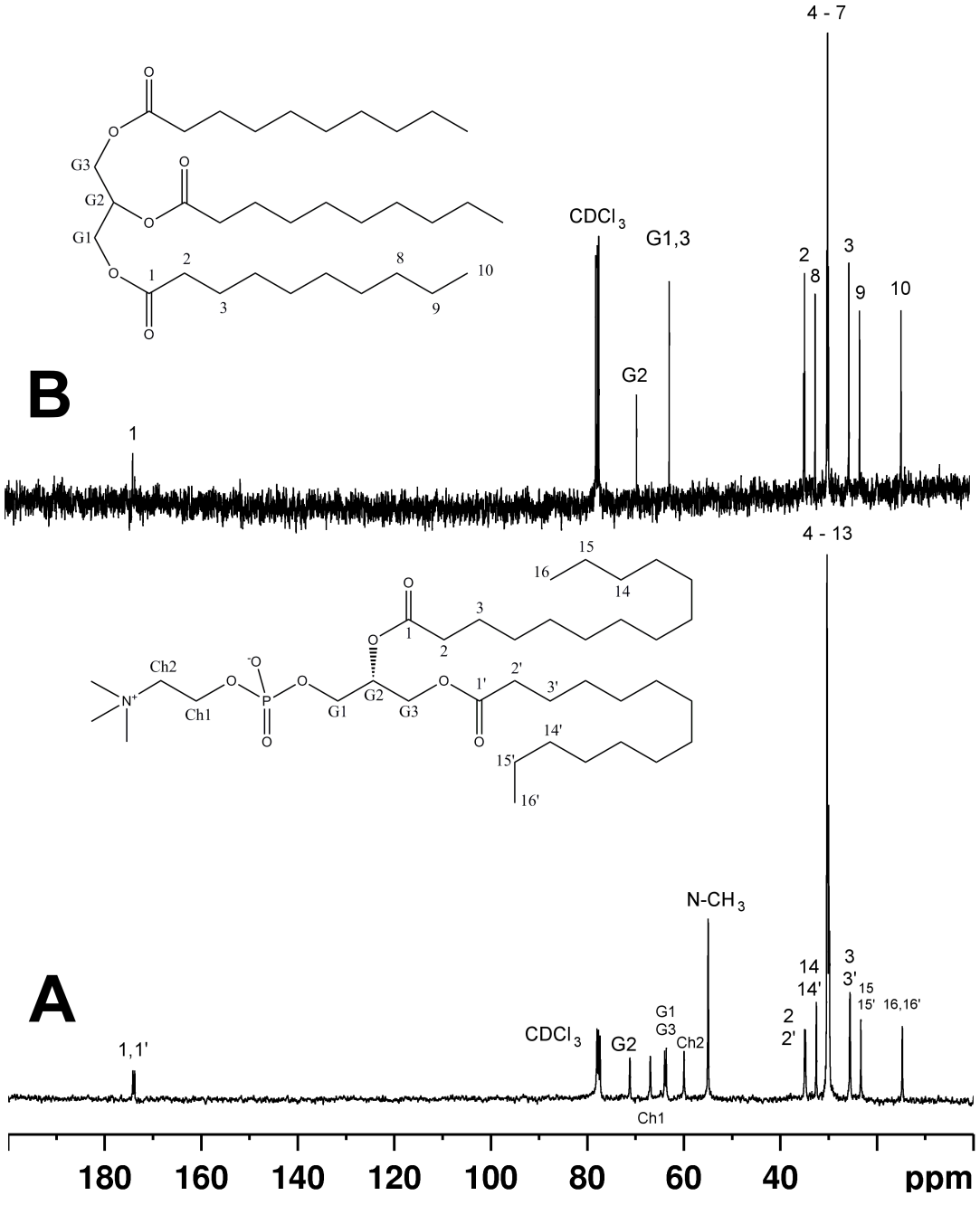
Supplemental V ^{13}C solid state NMR spectra of: A - solid cholesterol, and B – solid cholesteryl palmitate (both samples run as purchased). Note that, because of slight differences in atomic environment imposed by molecular conformational, packing, and crystal polymorphism effects, otherwise chemically identical carbon atoms can give rise to more than one signal. In favourable cases the solid state NMR spectrum can be used to identify known crystal forms.



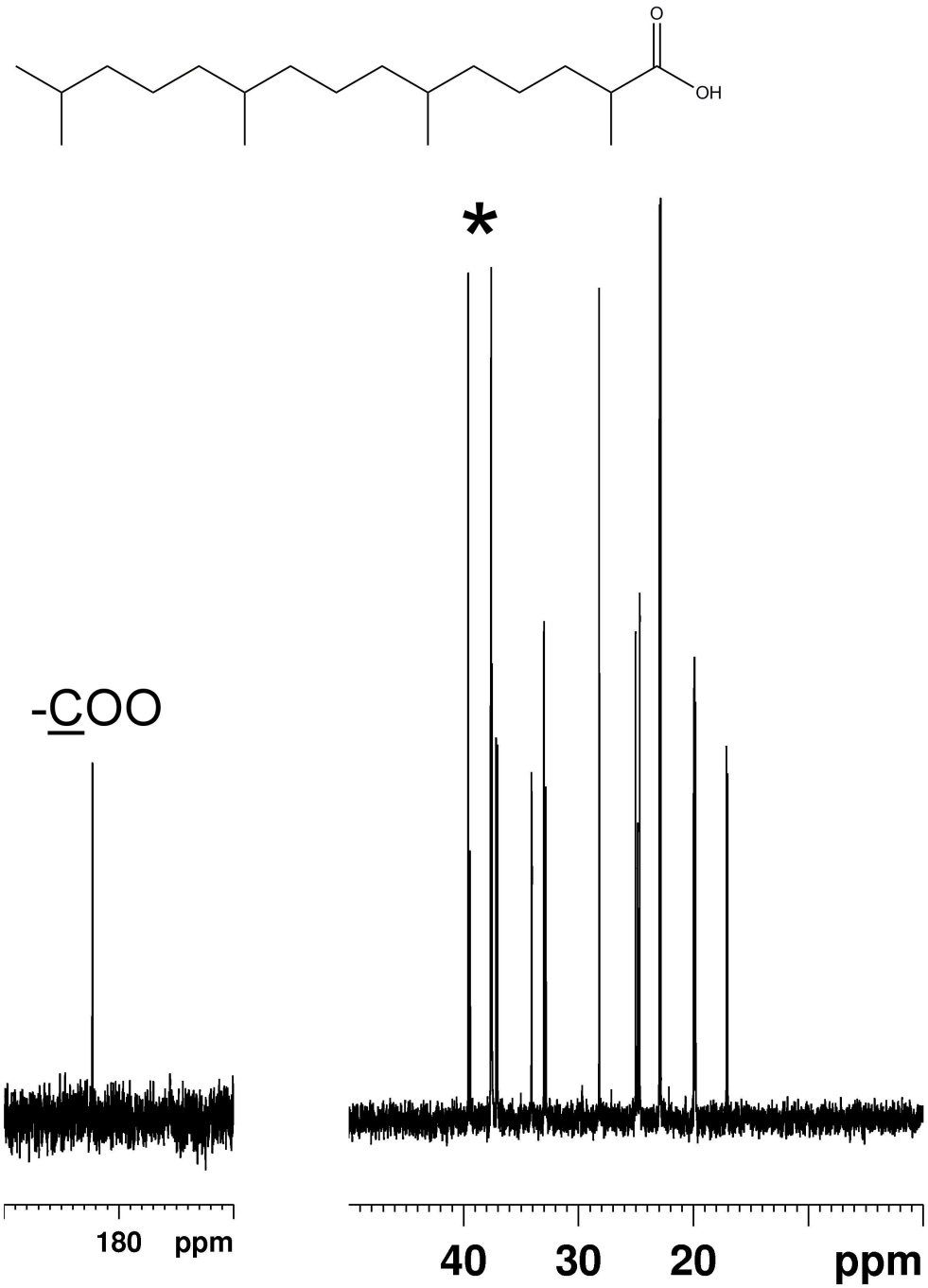
Supplemental VI ^{13}C solid state NMR spectra of: A – solid synthetic dimyristoylphosphatidylcholine (DMPC) (myristic acid = tetradecanoic acid), and B – solid phosphatidylserine (PS) from bovine brain. Note that the pure DMPC gives rise to a number of distinct signals for many chemically identical carbons, for the same reasons as discussed in Supplemental 5. Note also the broadness of the signals from the natural PS on account of chemical heterogeneity as well as differential molecular packing effects.



Supplemental VII ^{13}C solution state NMR spectra (in $CDCl_3$) of: A – cholesterol, and B – cholesteryl oleate, a model of a typical natural cholesteryl ester. The dashed red lines convey that the signals from the 5- and 6-carbon atoms of the cholesterol ring are useful markers of the whether the ring is free or esterified.



Supplemental VIII ^{13}C solution state NMR spectra (in $CDCl_3$) of: A – DMPC, and B – tridecanoyl glycerate.



Supplemental IX ^{13}C solution state NMR spectra (in $CDCl_3$) of pristanic acid. The asterisk marks signals from methylated carbons.