

Supplementary Materials

Article

Biocatalytic Insights for The Synthesis of New Prodrugs: Design of two Ibuprofen Derivatives

Federico Zappaterra, Francesco Presini, Valentina Venturi, Lindomar Alberto Lerin, Pier Paolo Giovannini and Stefania Costa

PROTON_01FZ69_mono

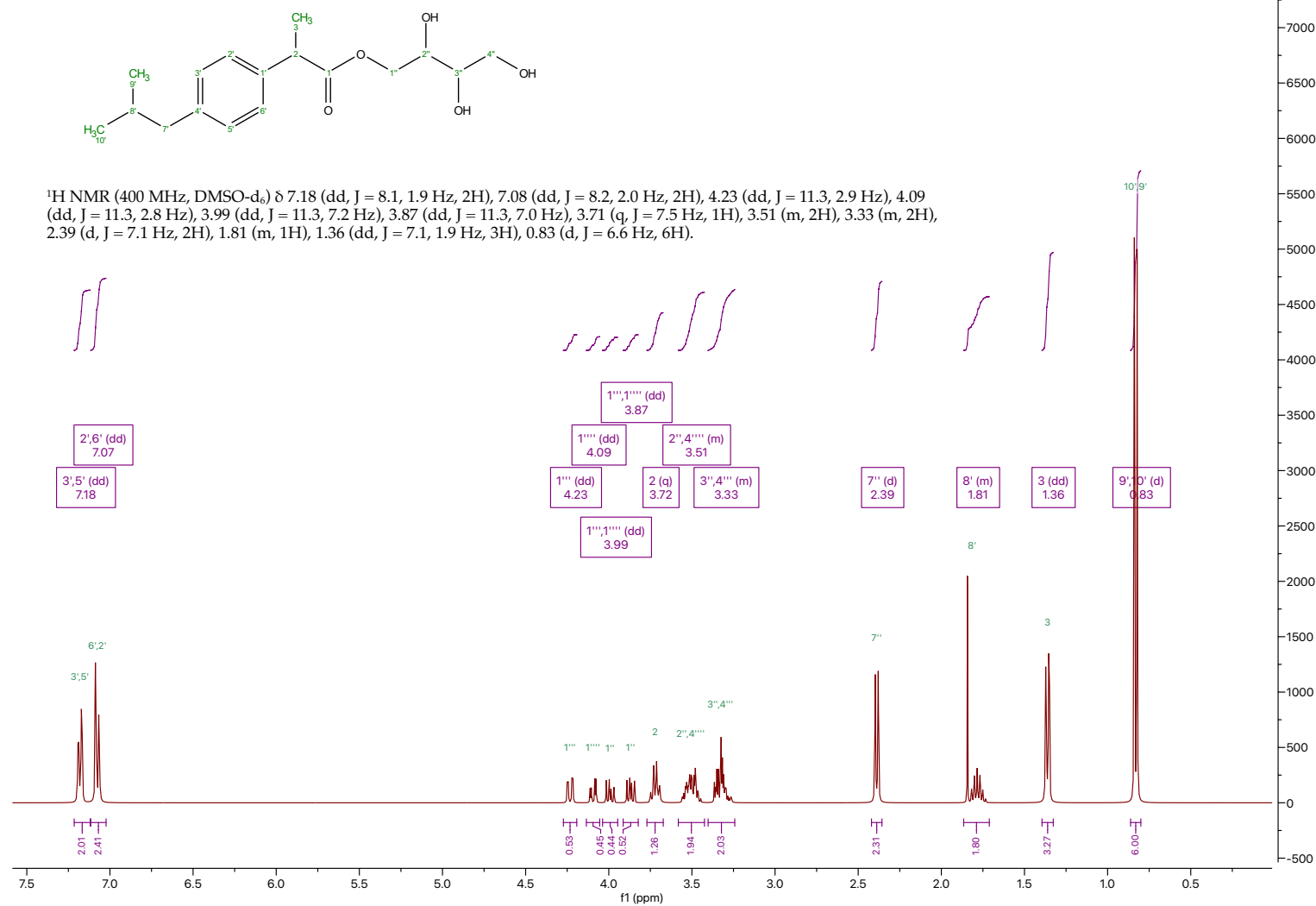


Figure S1: ¹H-NMR of erythritol ester of ibuprofen (**3a/3b**).

CARBON_01FZ69_mono

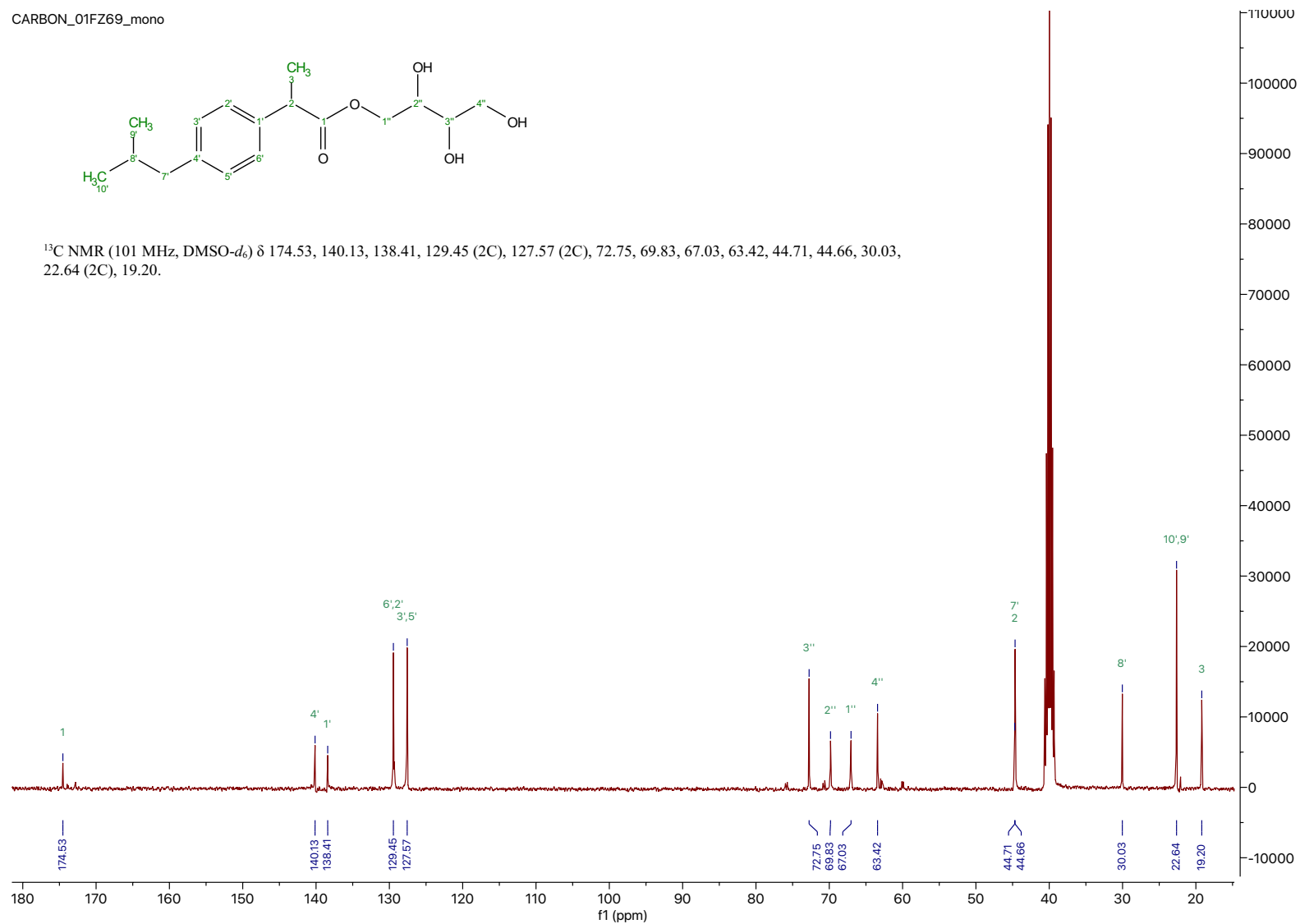


Figure S2: ¹³C-NMR of erythritol ester of ibuprofen (**3a/3b**).

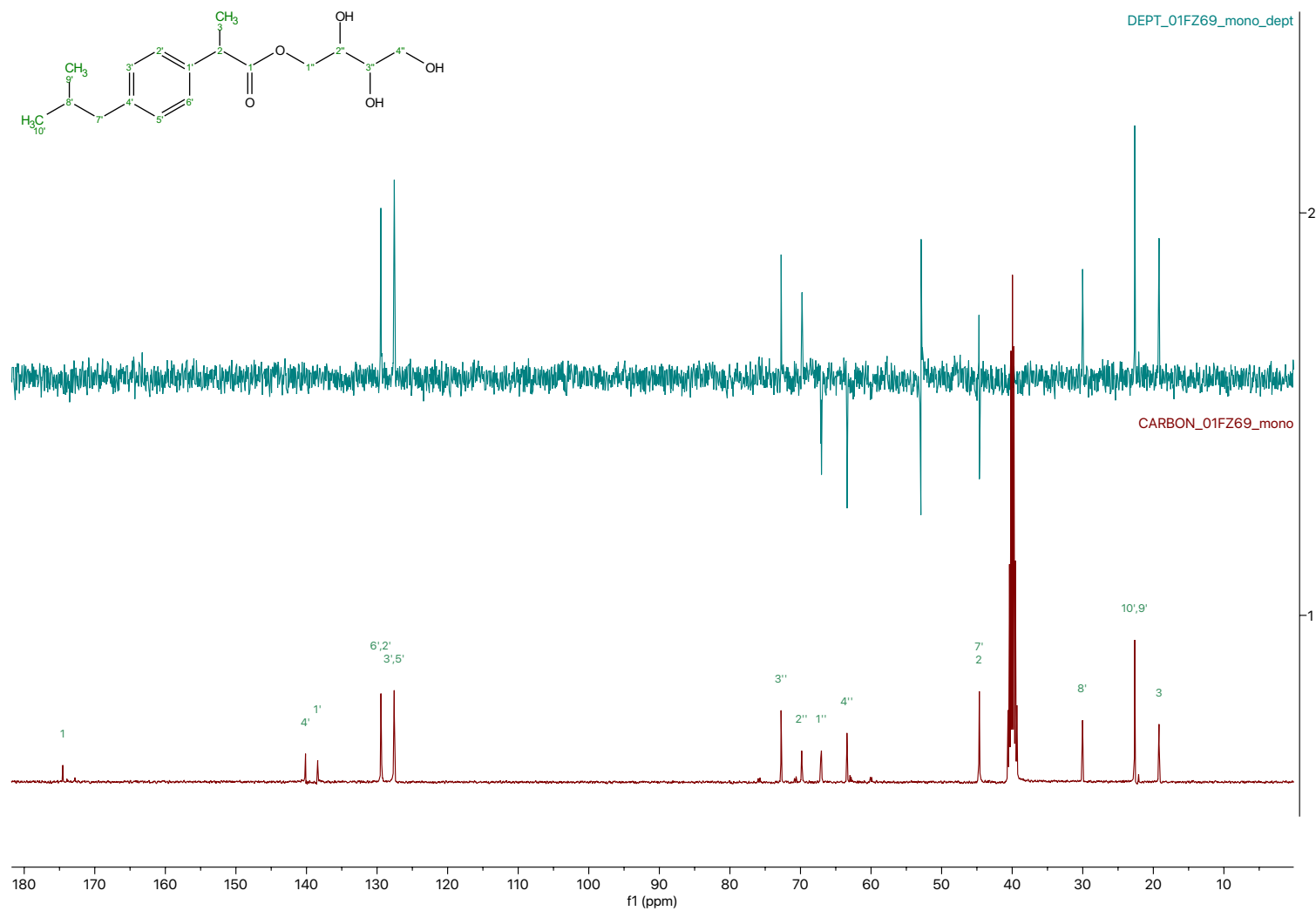


Figure S3: DEPT-NMR of erythritol ester of ibuprofen (3a/3b).

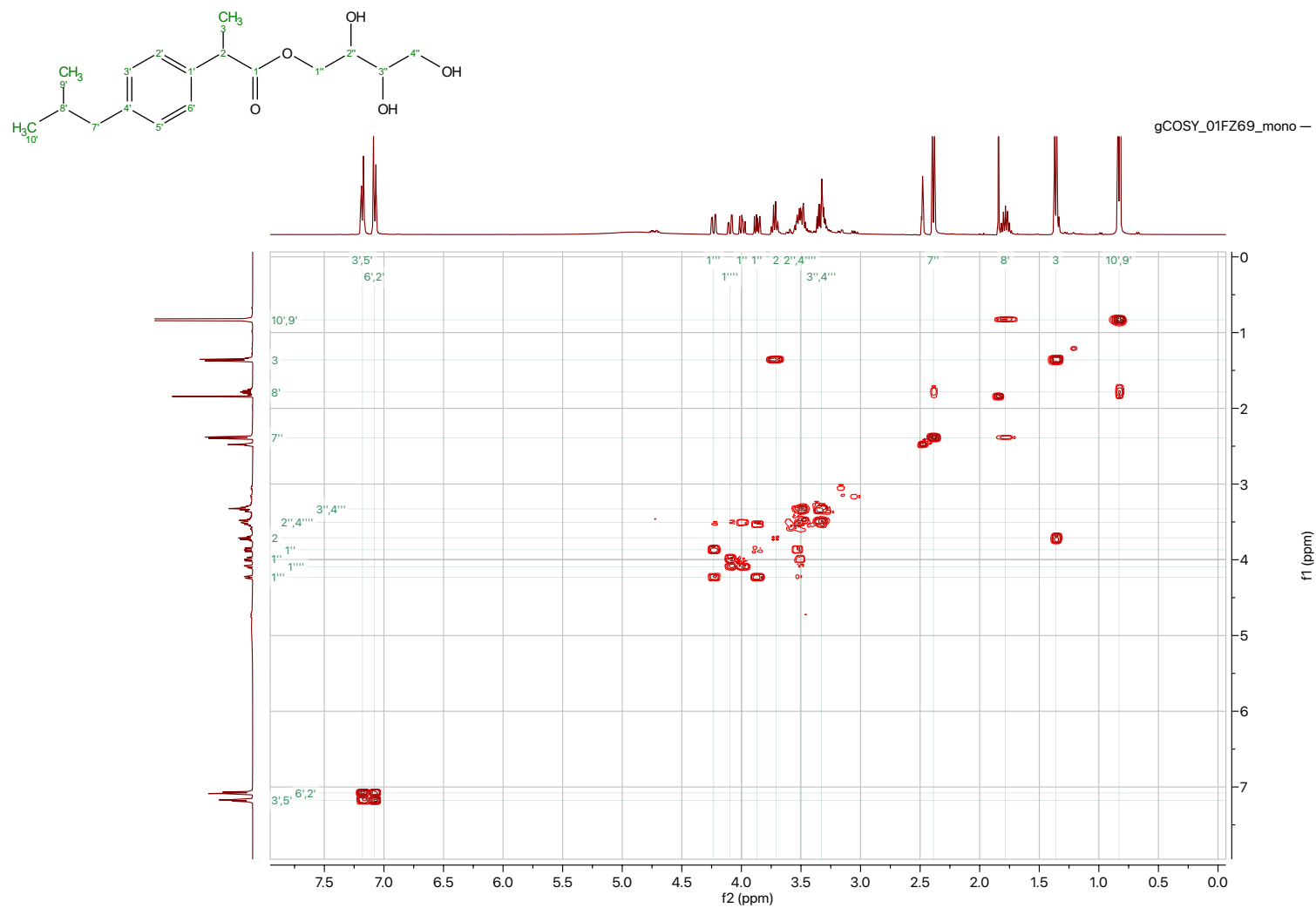


Figure S4: COSY-NMR of erythritol ester of ibuprofen (3a/3b).

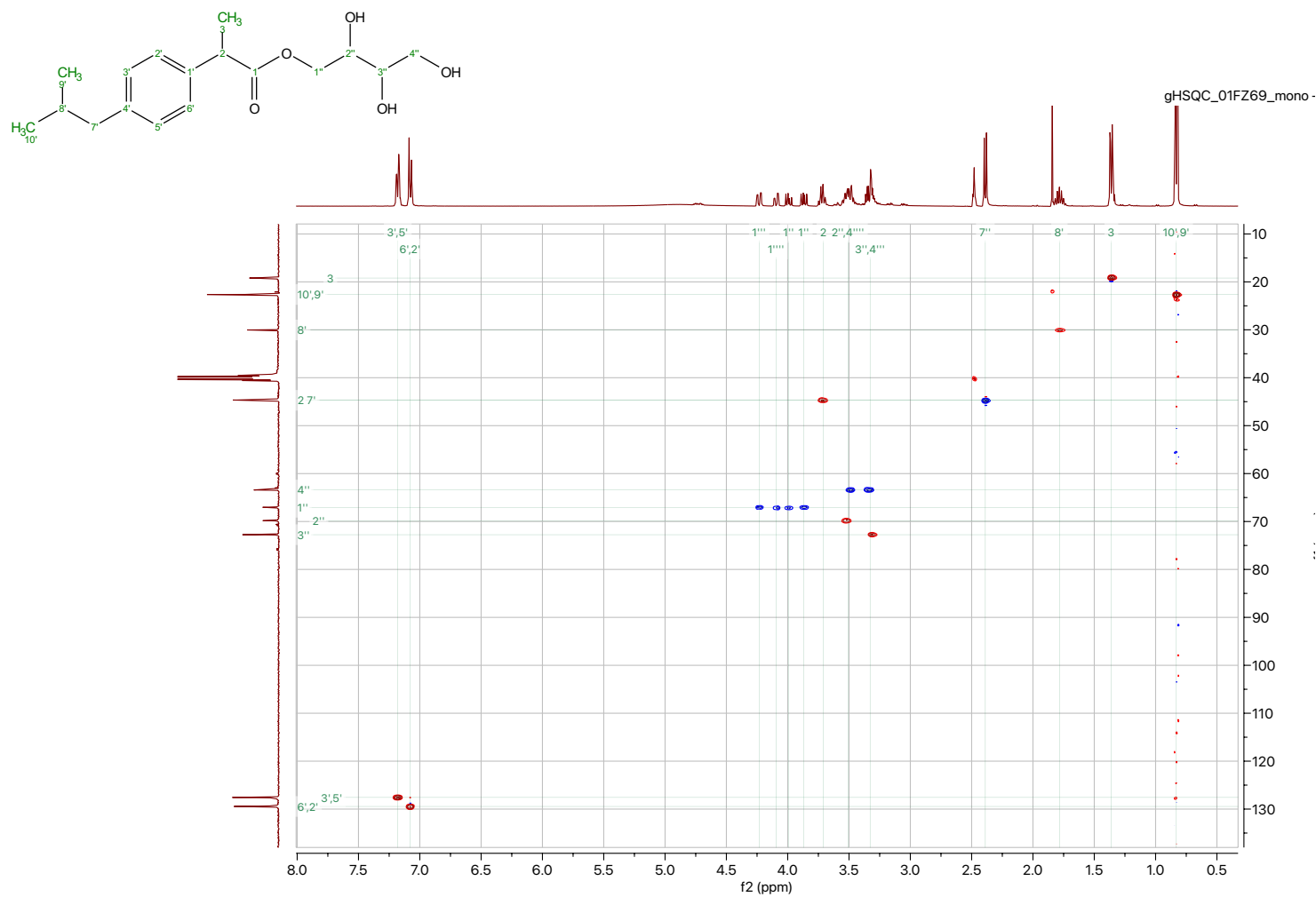


Figure S5: HSQC-NMR of erythritol ester of ibuprofen (3a/3b).

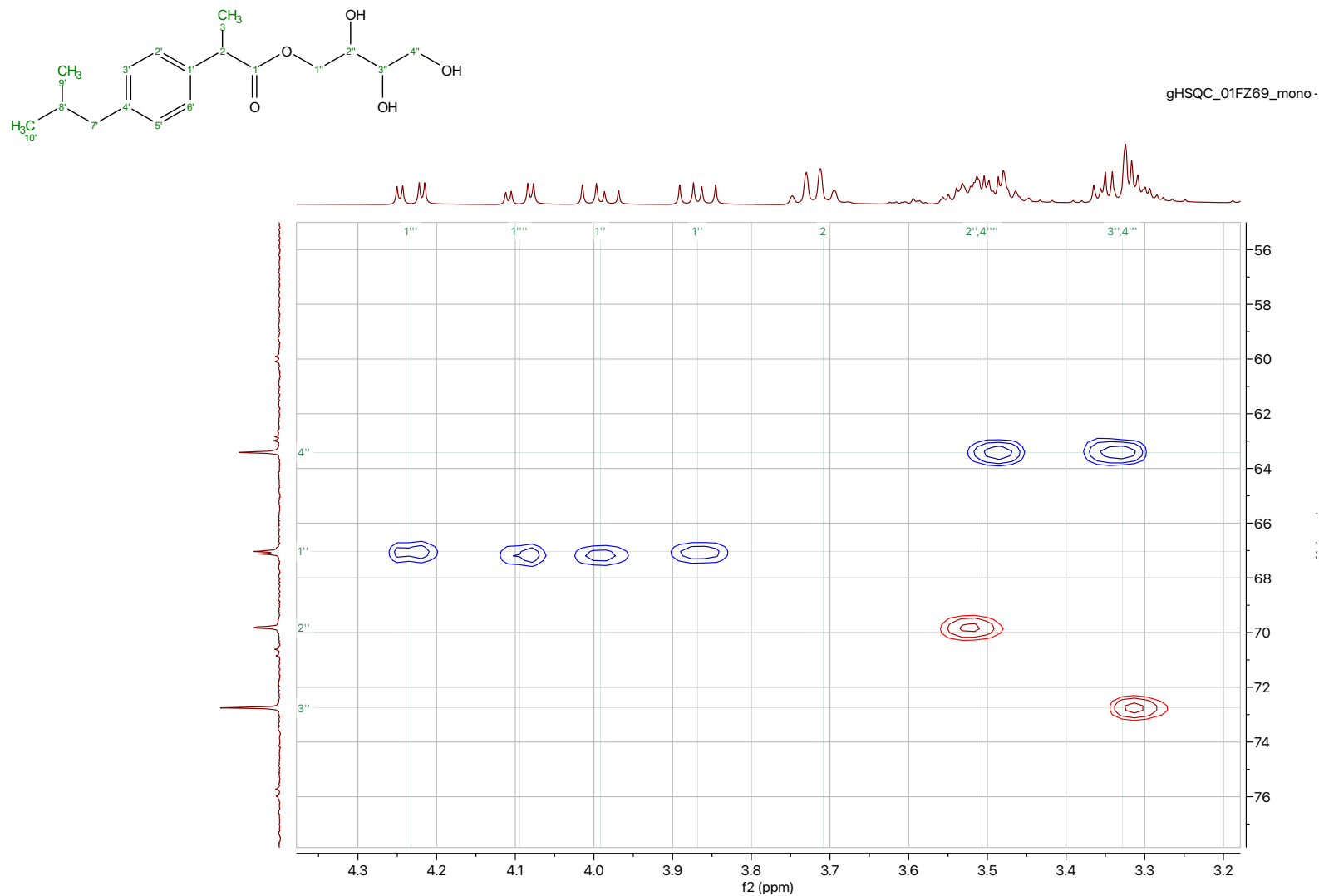


Figure S6: Zoom of the HSQC-NMR of erythritol ester of ibuprofen (3a/3b).

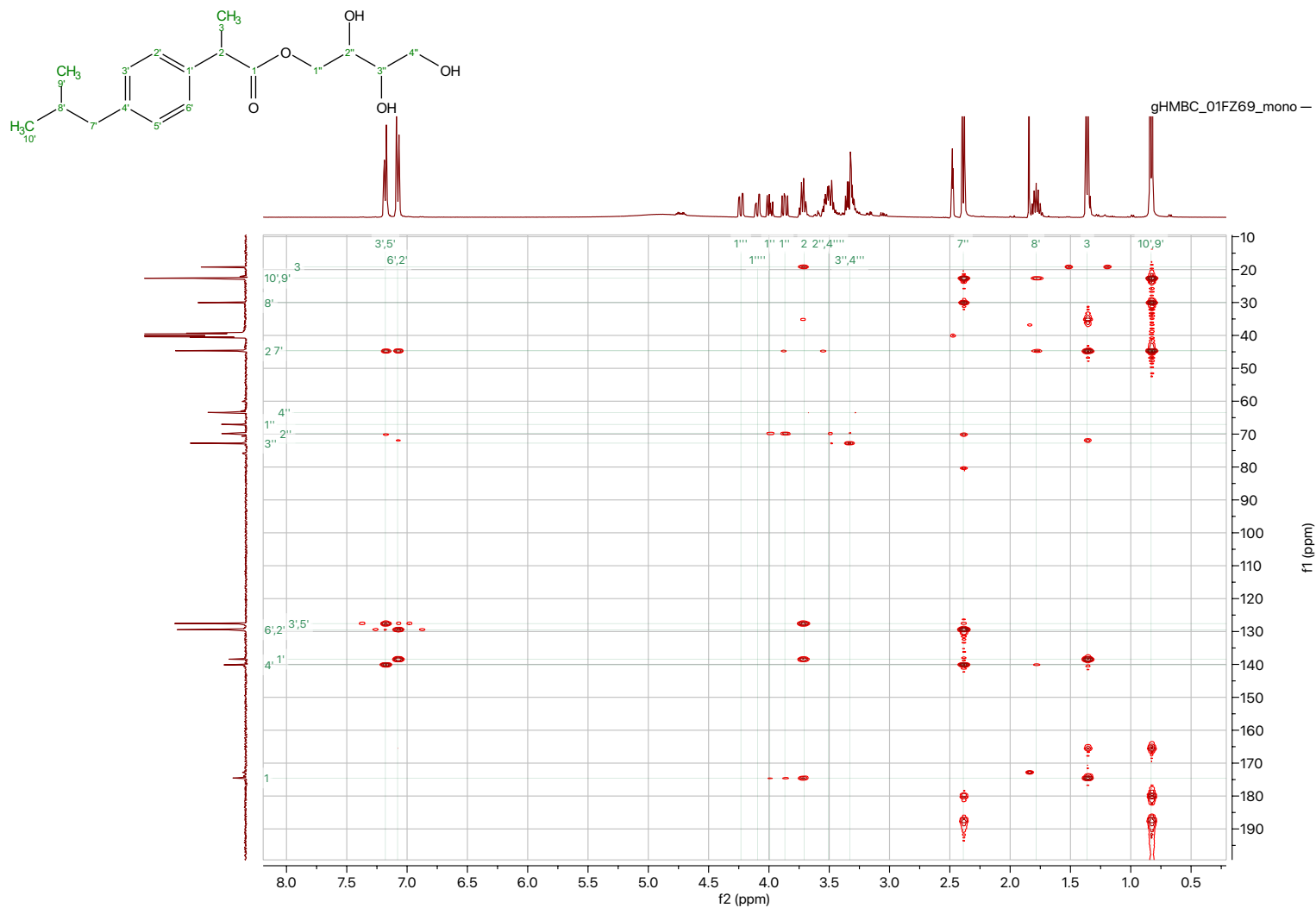


Figure S7: HMBC-NMR of erythritol ester of ibuprofen (3a/3b).

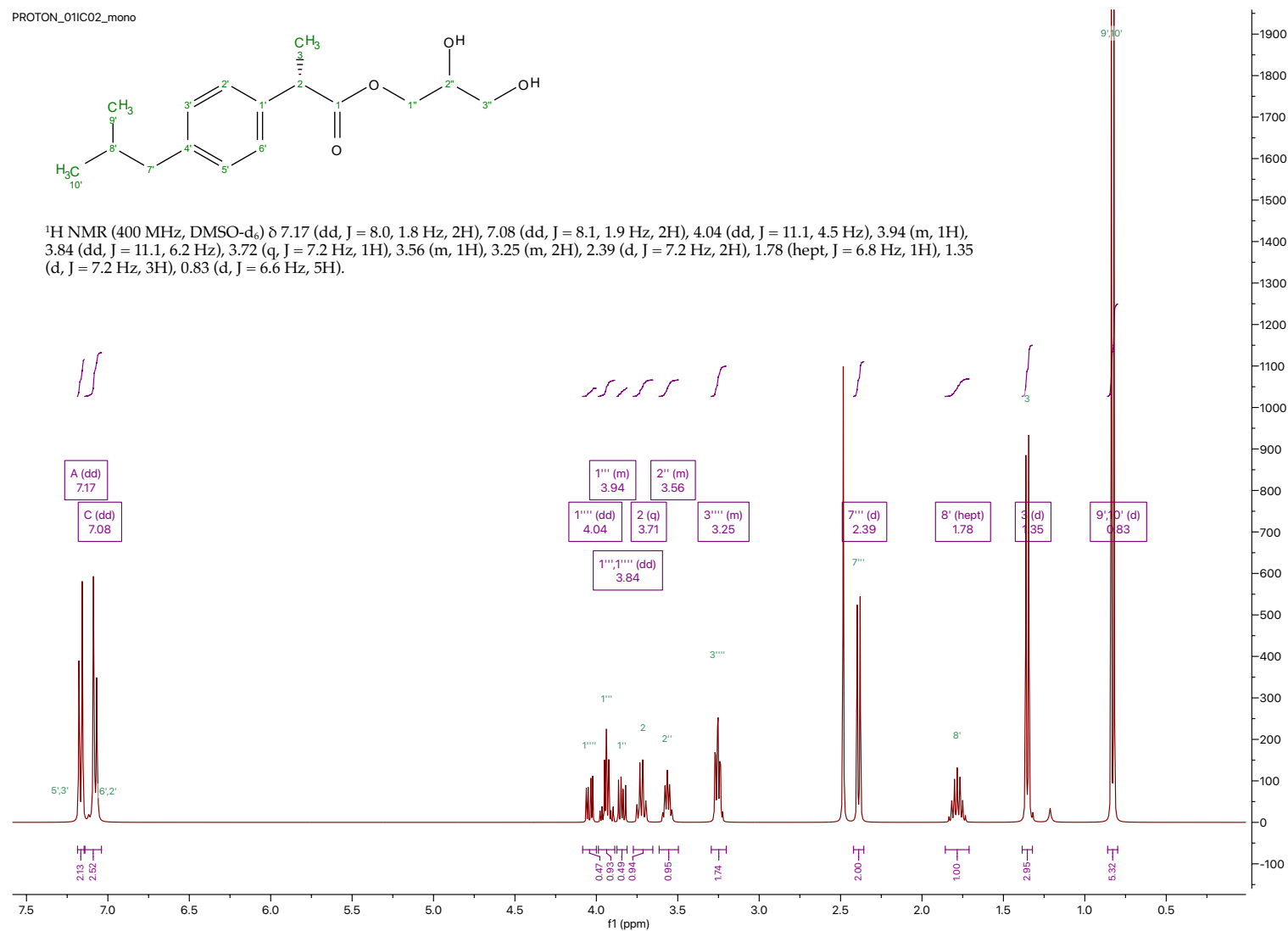
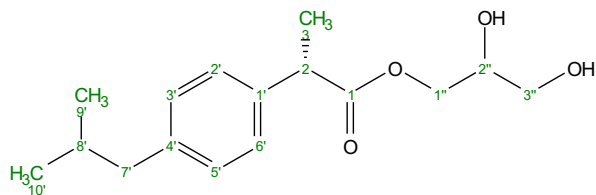


Figure S8: ¹H-NMR of glycerol ester of ibuprofen (**6a/6b**).

PROTON_01IC02_mono



^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 7.17 (d, 2H), 7.08 (d, 2H), 4.04 – 3.84 (dd, $J = 11.1, 4.5$ Hz; m; dd, $J = 11.1, 6.2$ Hz, 3H) 3.72 (q, $J = 7.2$ Hz, 1H), 3.56 (p, $J = 5.6$ Hz, 1H), 3.29 – 3.20 (m, 2H), 2.39 (d, $J = 7.2$ Hz, 2H), 1.78 (hept, $J = 6.8$ Hz, 1H), 1.35 (d, $J = 7.2$ Hz, 3H), 0.83 (d, $J = 6.6$ Hz, 5H).

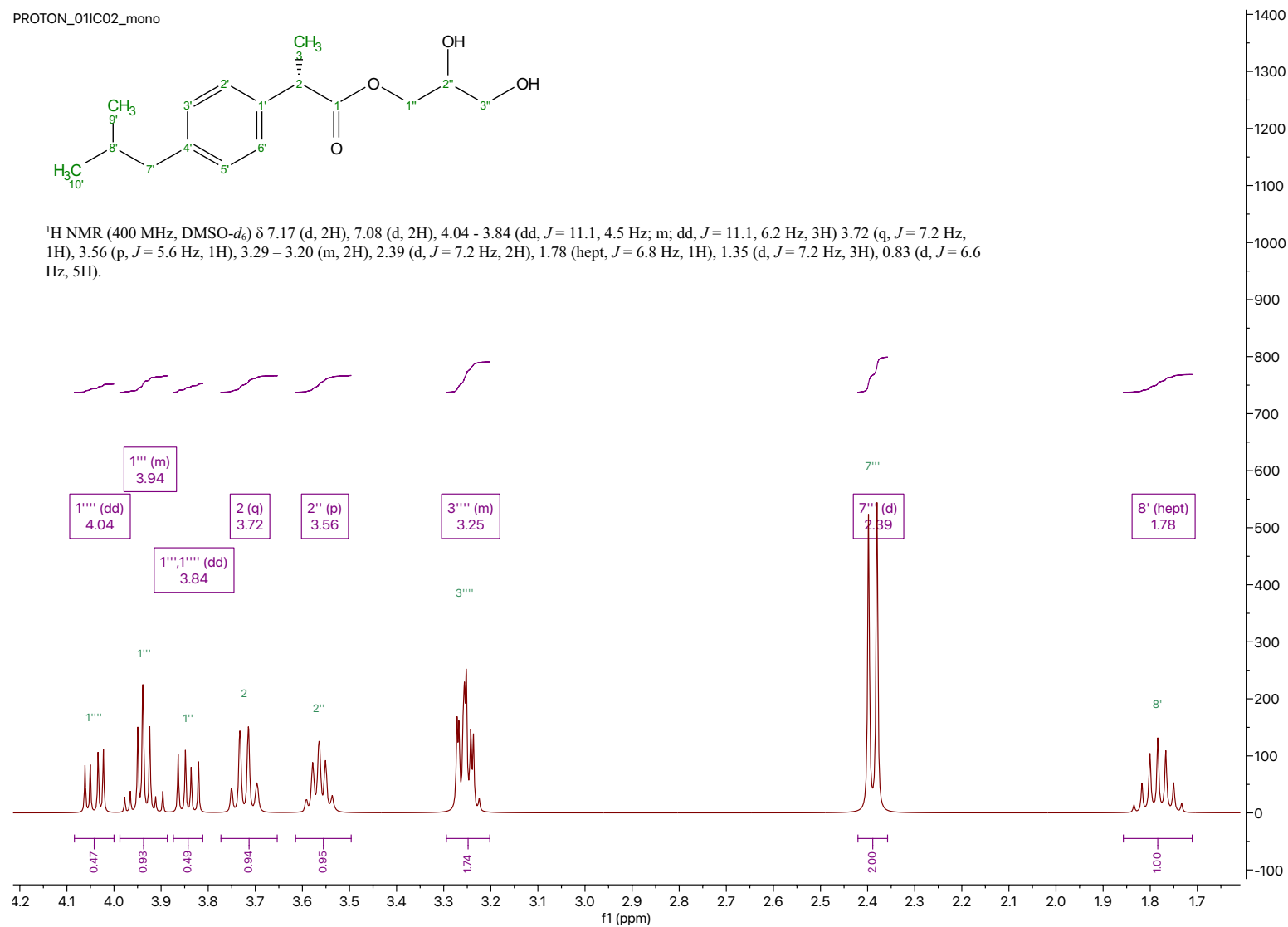


Figure S9: Zoom of the ^1H -NMR of glycerol ester of ibuprofen (**6a/6b**).

CARBON_01IC02_mono

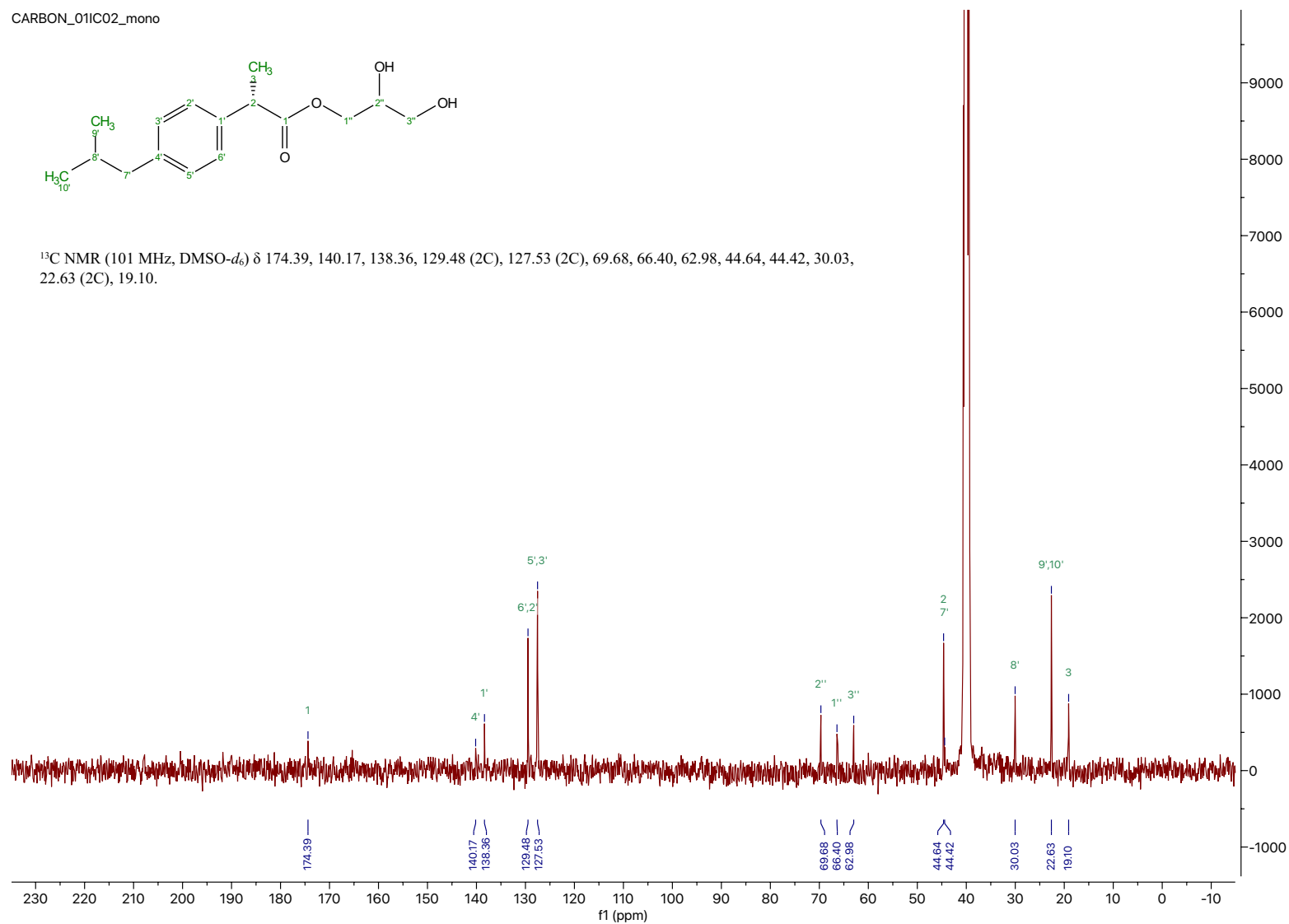


Figure S10: ¹³C-NMR of glycerol ester of ibuprofen (6a/6b).

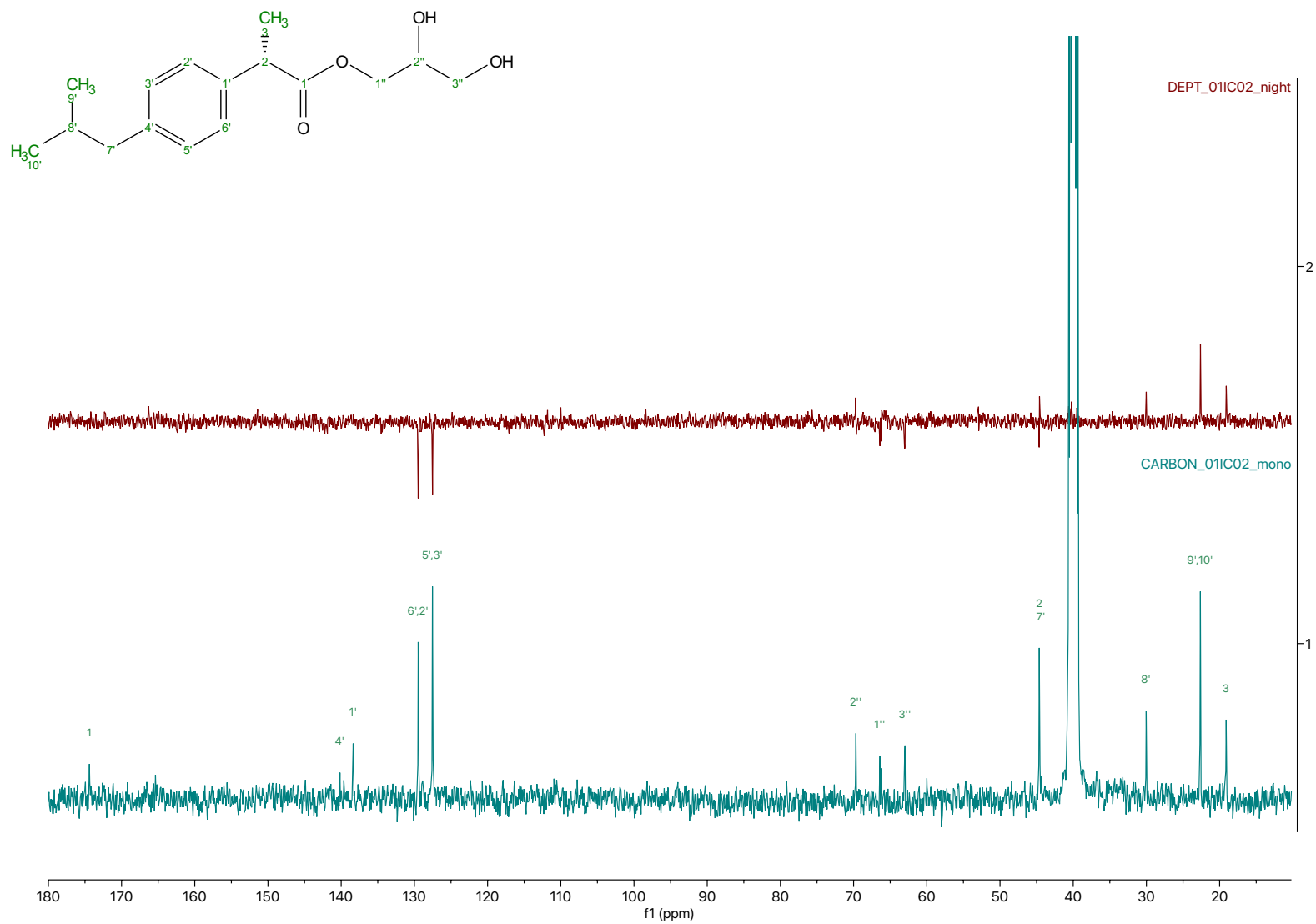


Figure S11: DEPT-NMR of glycerol ester of ibuprofen (**6a/6b**).

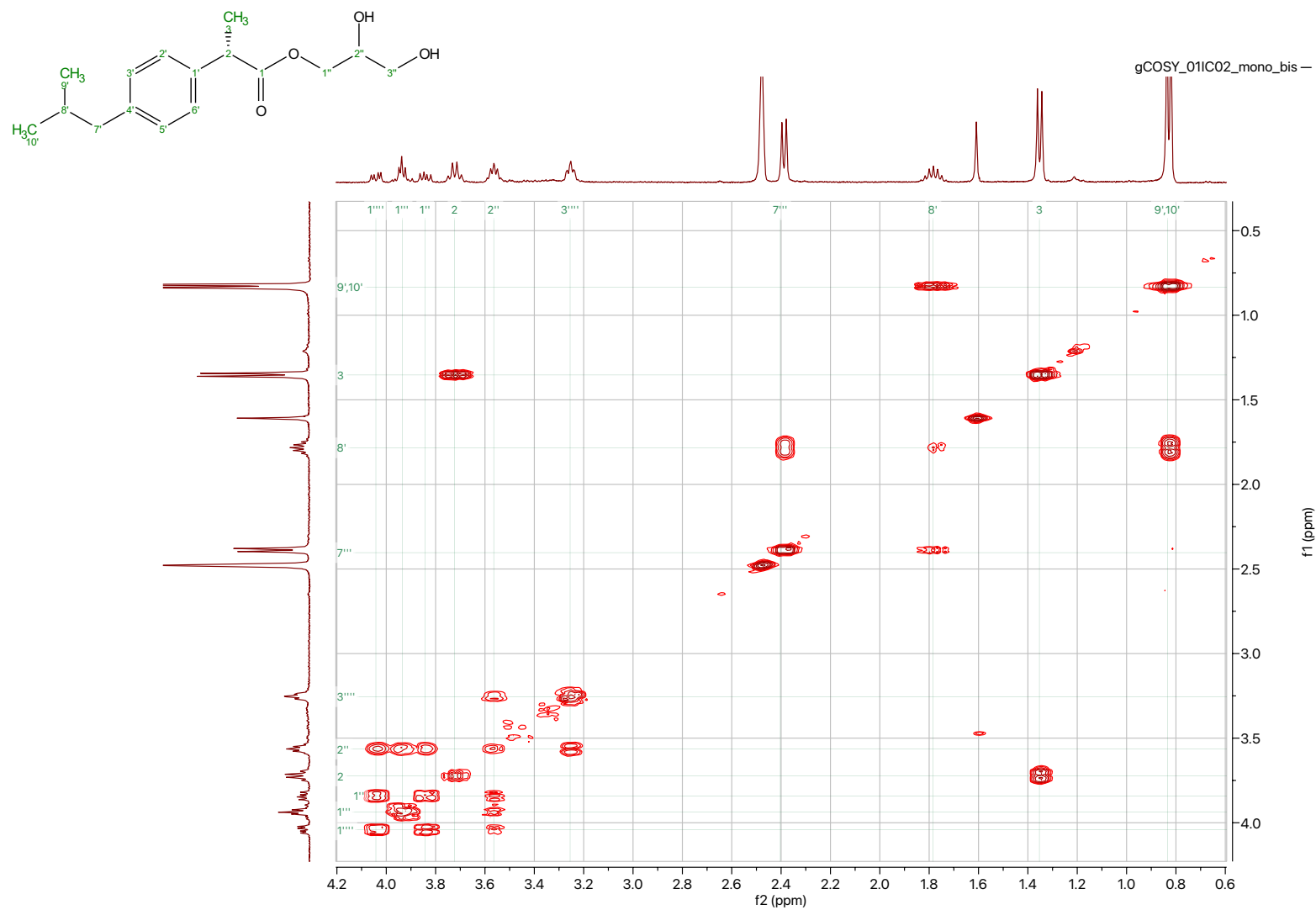


Figure S13: Zoom of the COSY-NMR of glycerol ester of ibuprofen (6a/6b).

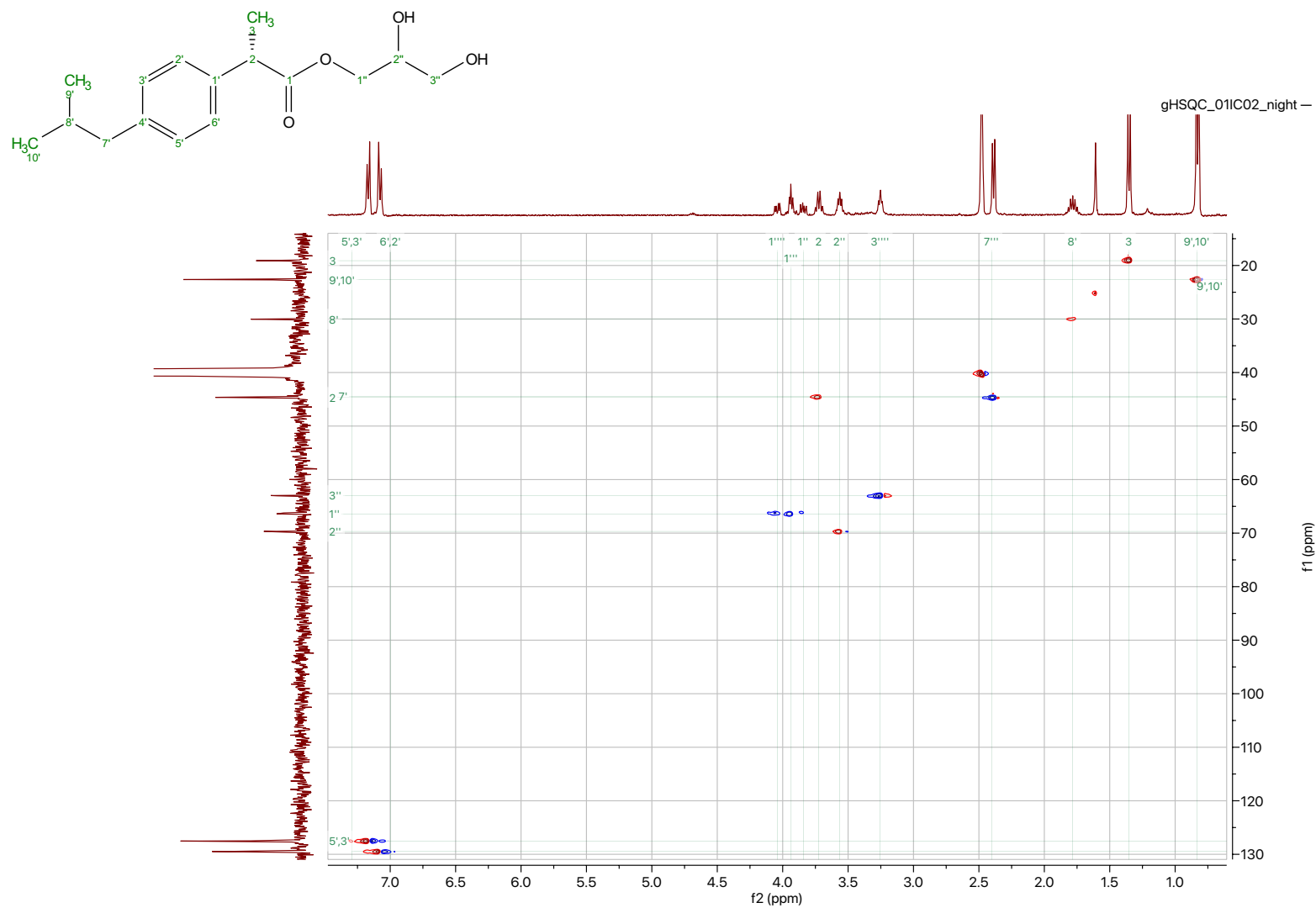


Figure S14: HSQC-NMR of glycerol ester of ibuprofen (**6a/6b**).

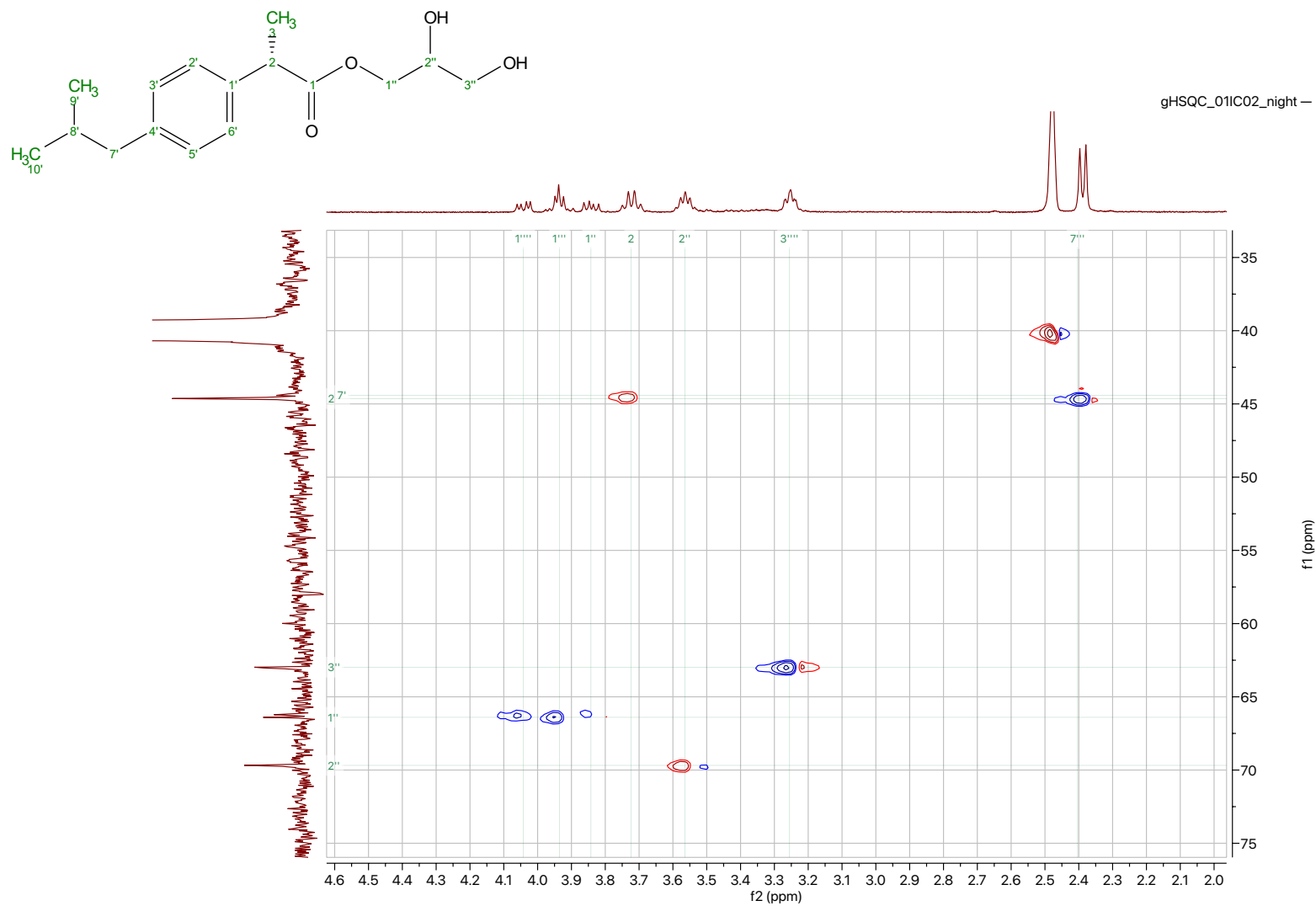


Figure S15: Zoom of the HSQC-NMR of glycerol ester of ibuprofen (**6a/6b**).

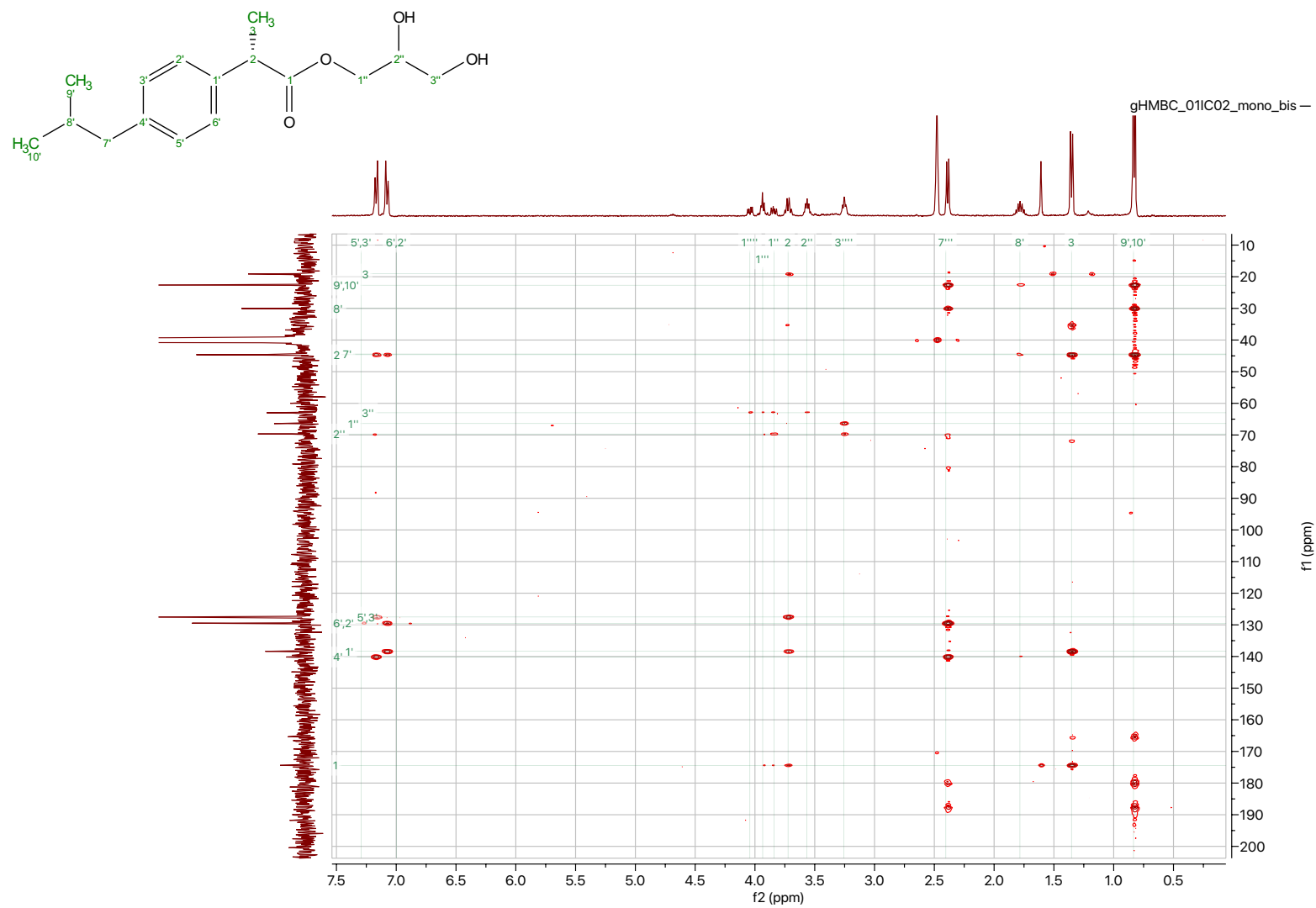


Figure S16: HMBC-NMR of glycerol ester of ibuprofen (**6a/6b**).

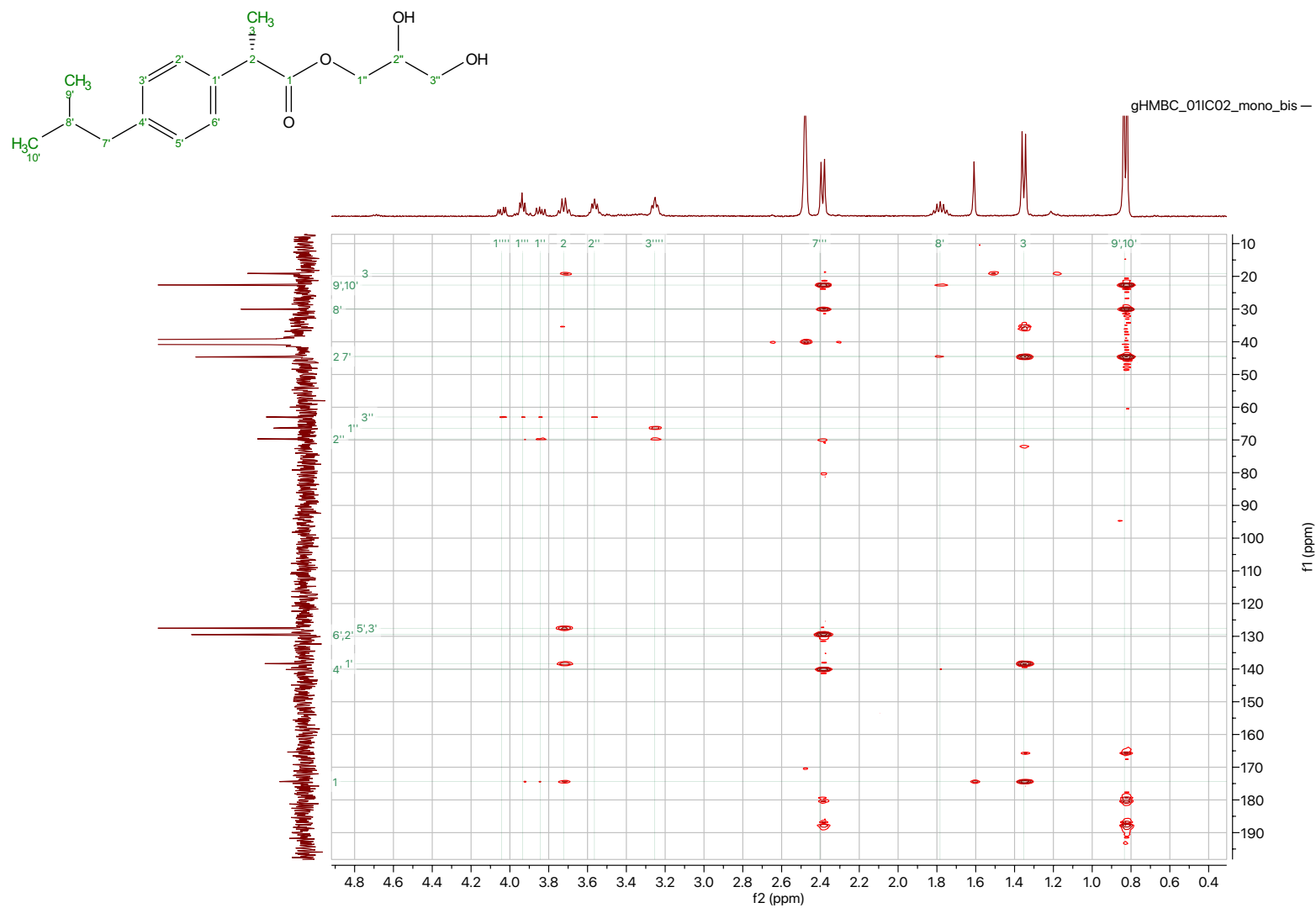


Figure S17: Zoom of the HMBC-NMR of glycerol ester of ibuprofen (**6a/6b**).

FZ68_Rf04_D2O_2-1H —

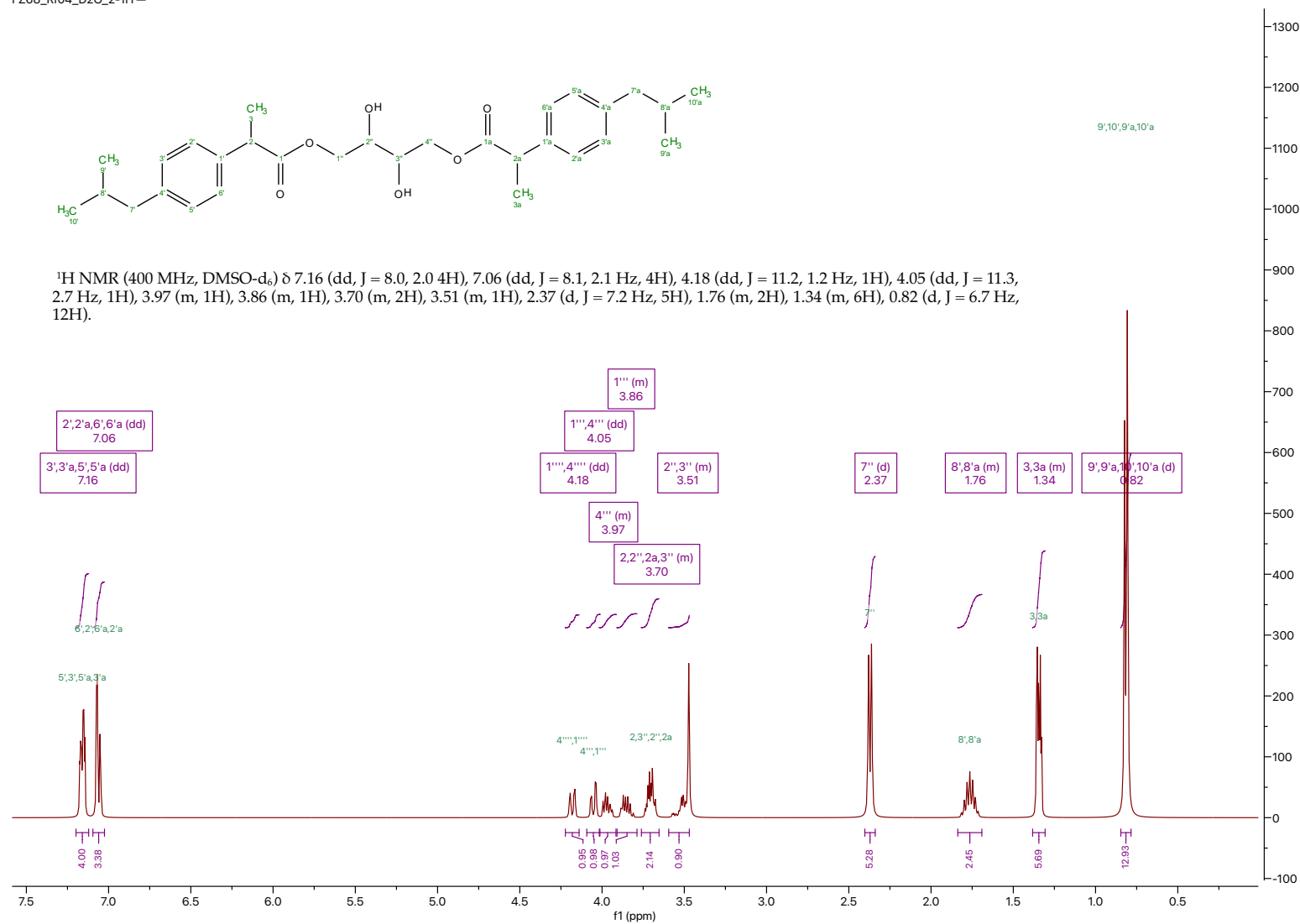


Figure S18: ¹H-NMR of the diacylated erythritol ester of ibuprofen (**4**).

CARBON_01

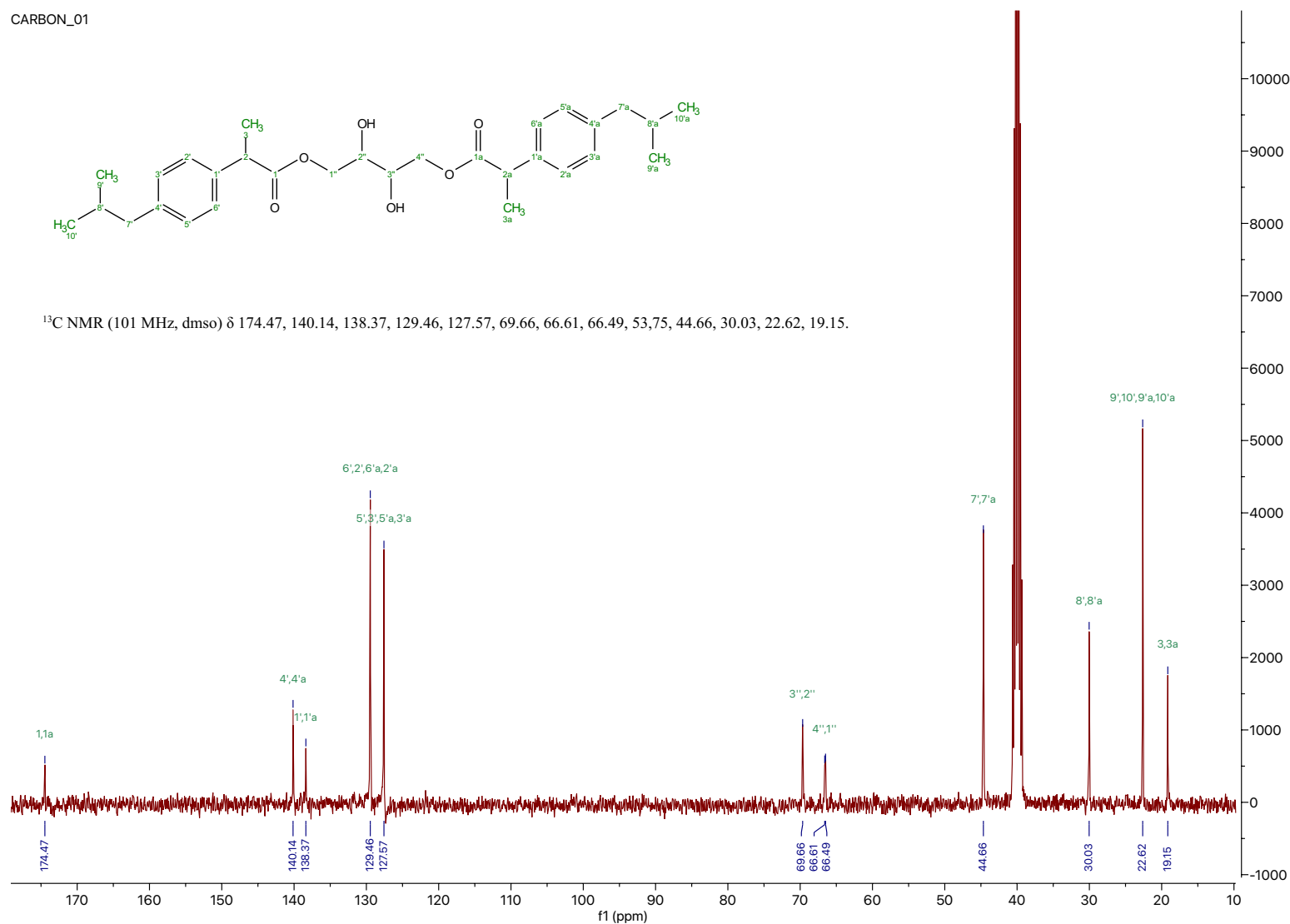


Figure S19: ¹³C-NMR of the diacylated erythritol ester of ibuprofen (**4**).

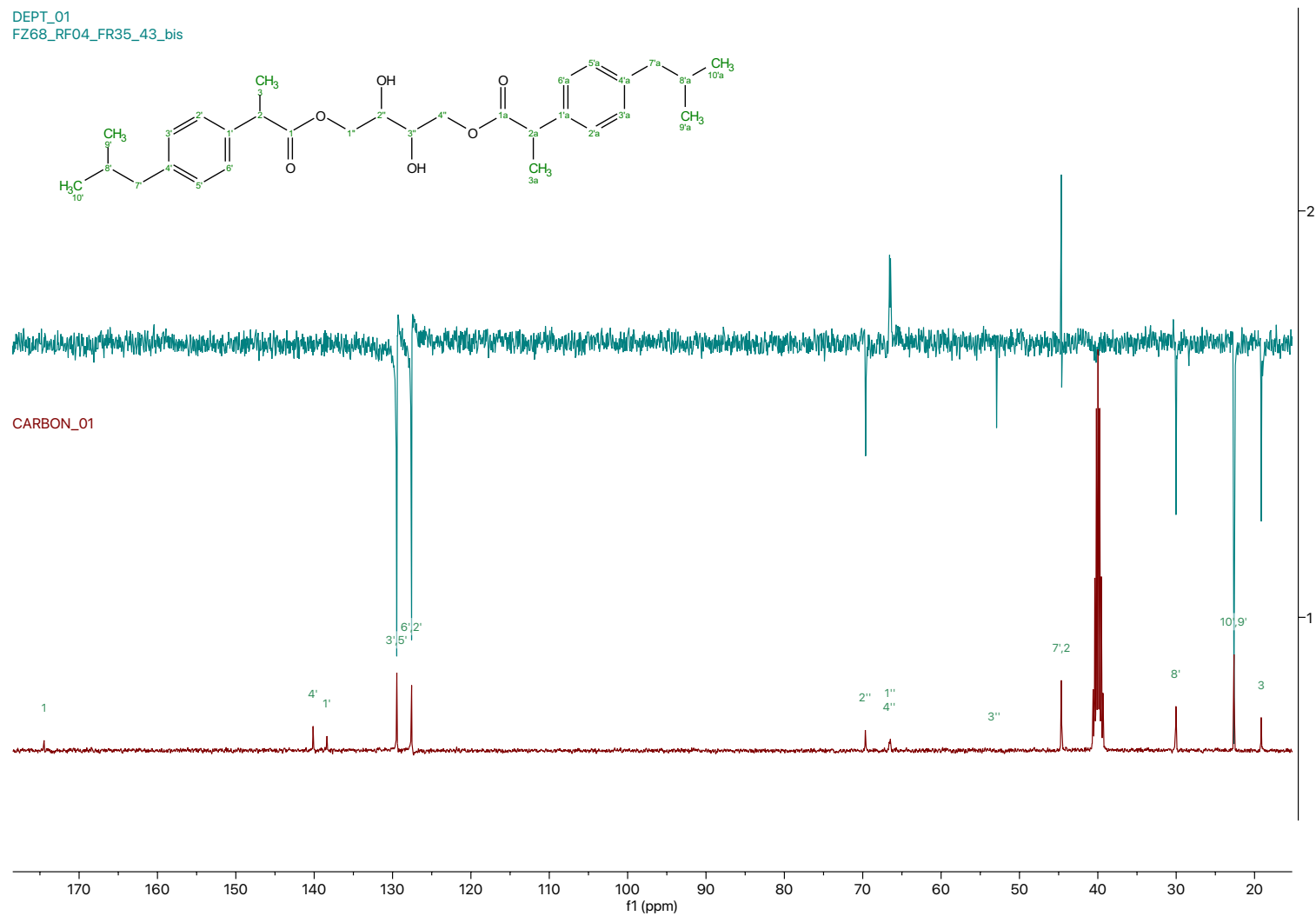


Figure S20: DEPT-NMR of the diacylated erythritol ester of ibuprofen (**4**).

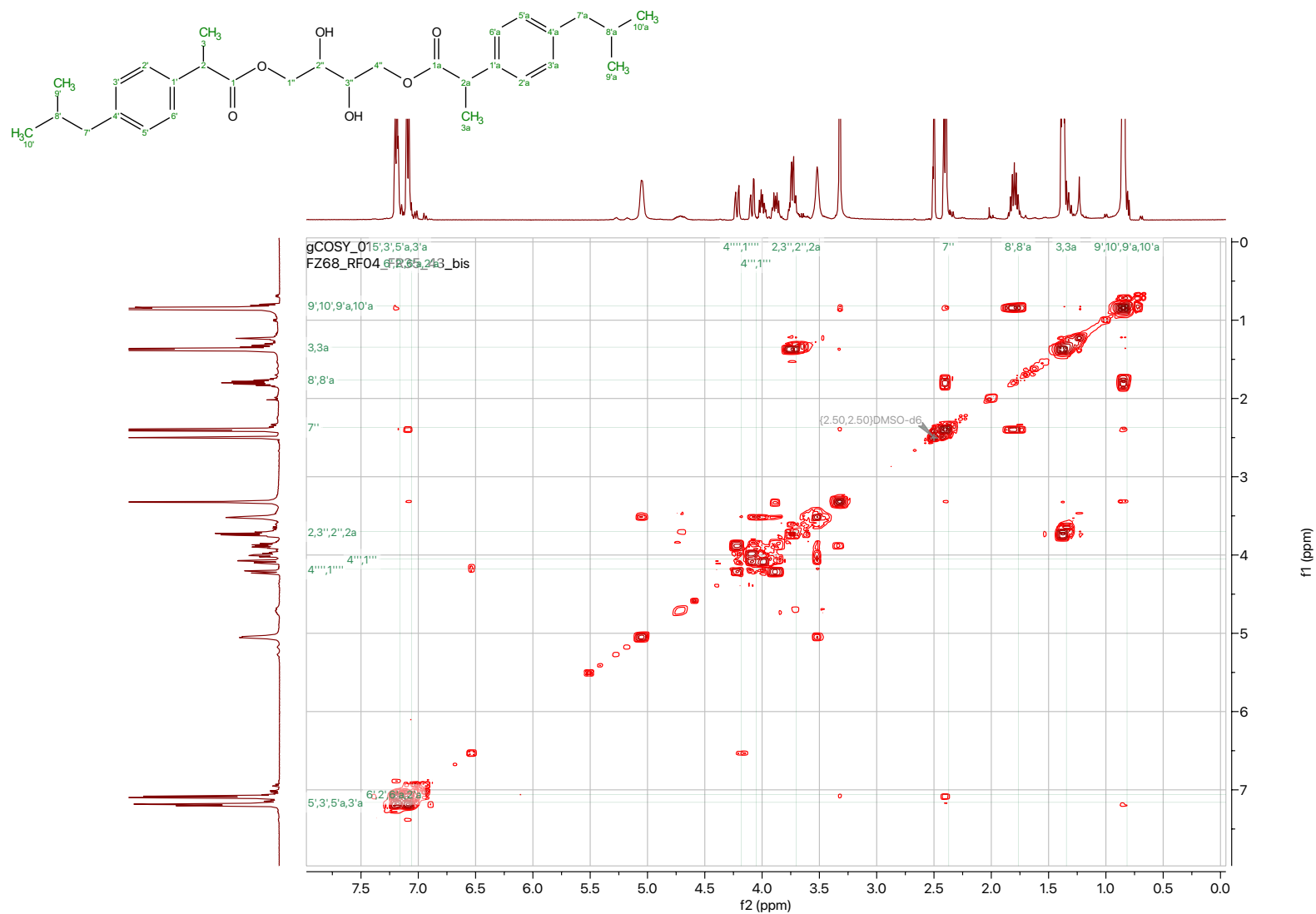


Figure S21: COSY-NMR of the diacylated erythritol ester of ibuprofen (4).

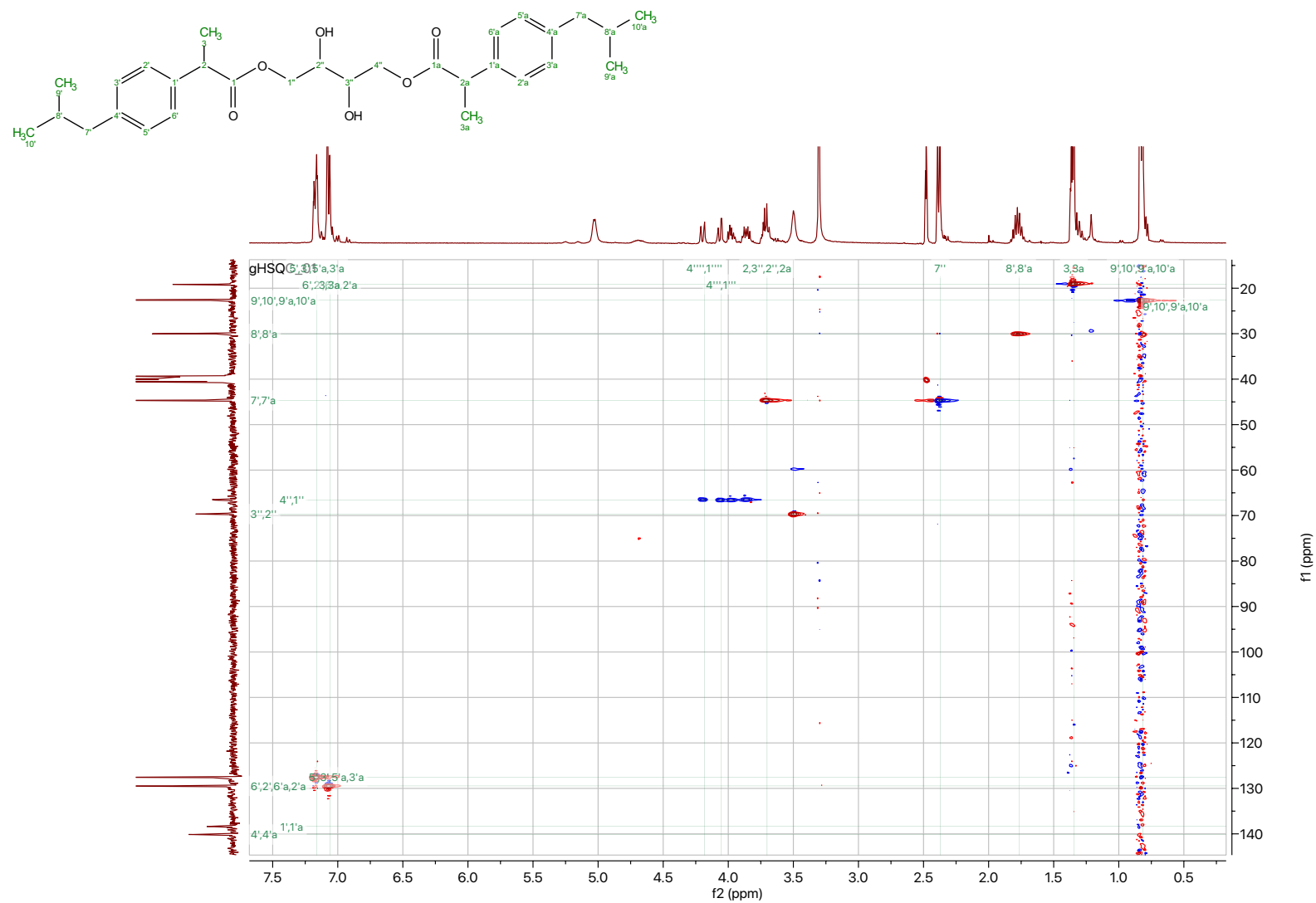


Figure S22: HSQC-NMR of the diacylated erythritol ester of ibuprofen (4).

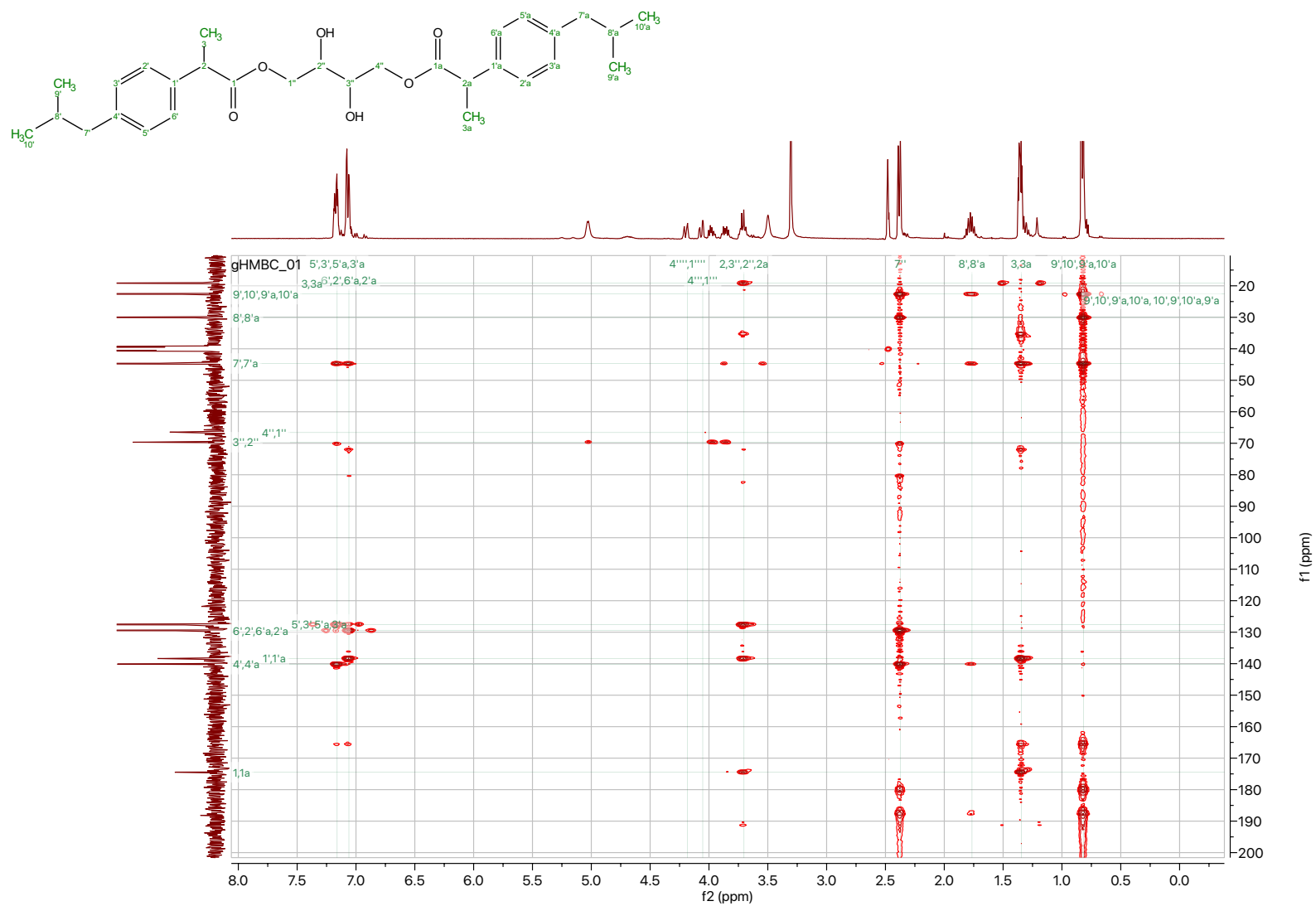


Figure S23: HMBC-NMR of the diacylated erythritol ester of ibuprofen (4).

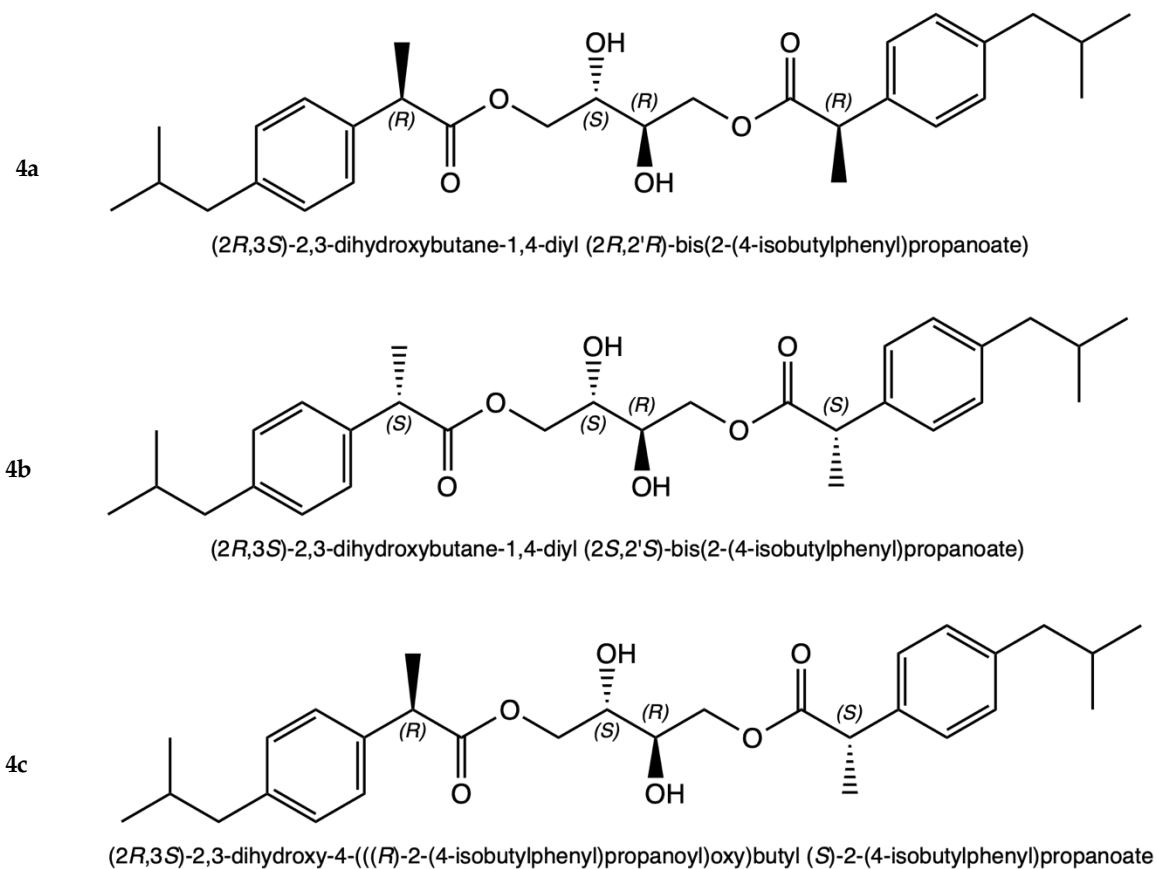


Figure S24: Representation of the three possible configurations of product **4** (**4a**, **4b**, and **4c**).