

SUPPORTING INFORMATION

Synthesis of zwitter-ionic conjugate of *nido*-carborane with cholesterol

Anna A. Druzina^{1,*}, Olga B. Zhidkova¹, Nadezhda V. Dudarova¹, Natalia A. Nekrasova^{1,2}, Kyrill Yu. Suponitsky^{1,3}, Sergey V. Timofeev¹ and Vladimir I. Bregadze¹

¹ A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov Str., 119991 Moscow, Russia; Zolga57@mail.ru (O.B.Z.); nadezjdino_96@mail.ru (N.V.D.); neksova_na@list.ru (N.A.N.); kirshik@yahoo.com (K.Yu.S.); timofeev@ineos.ac.ru (S.V.T.); bre@ineos.ac.ru (V.I.B).

² M.V. Lomonosov Institute of Fine Chemical Technology, MIREA - Russian Technological University, 86 Vernadsky Av., 119571, Moscow, Russia; neksova_na@list.ru (N.A.N.)

³ G.V. Plekhanov Russian University of Economics, 36 Stremyanniy Line, 117997, Moscow, Russia; kirshik@yahoo.com (K.Yu.S.)

* Correspondence: ilinova_anna@mail.ru; Tel.: +7-926-404-5566 (A.A.D.)

¹H, ¹¹B and ¹³C NMR, IR and high-resolution mass spectra of compounds **6**

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\INEOS\Laskova\da-041_&clb.d
Method tune_wide.m
Sample Name /CHIZ DA-041
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 29.09.2020 15:27:17

Operator BDAL@DE
Instrument maXis 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Waste

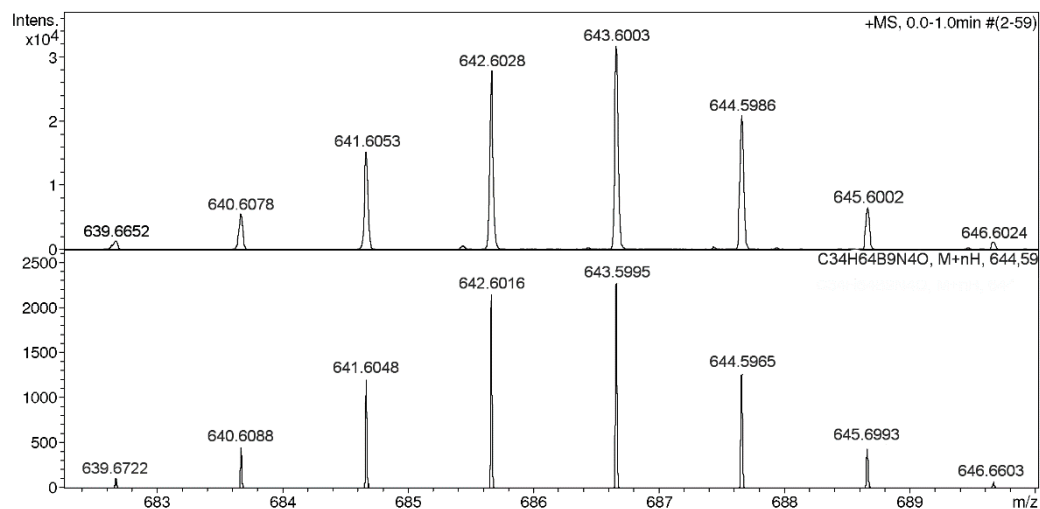
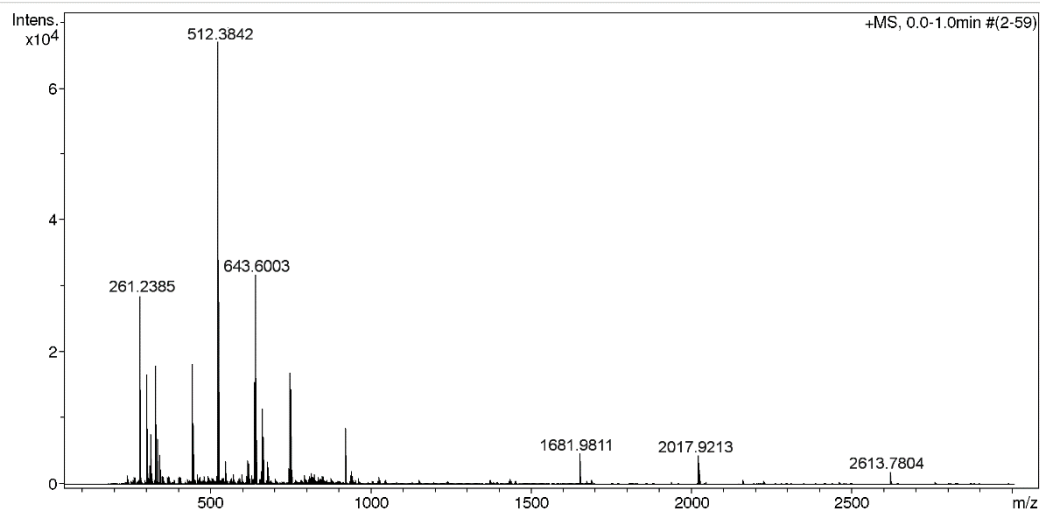


Figure S1. ESI-HRMS spectrum of compound 6

Compound 6

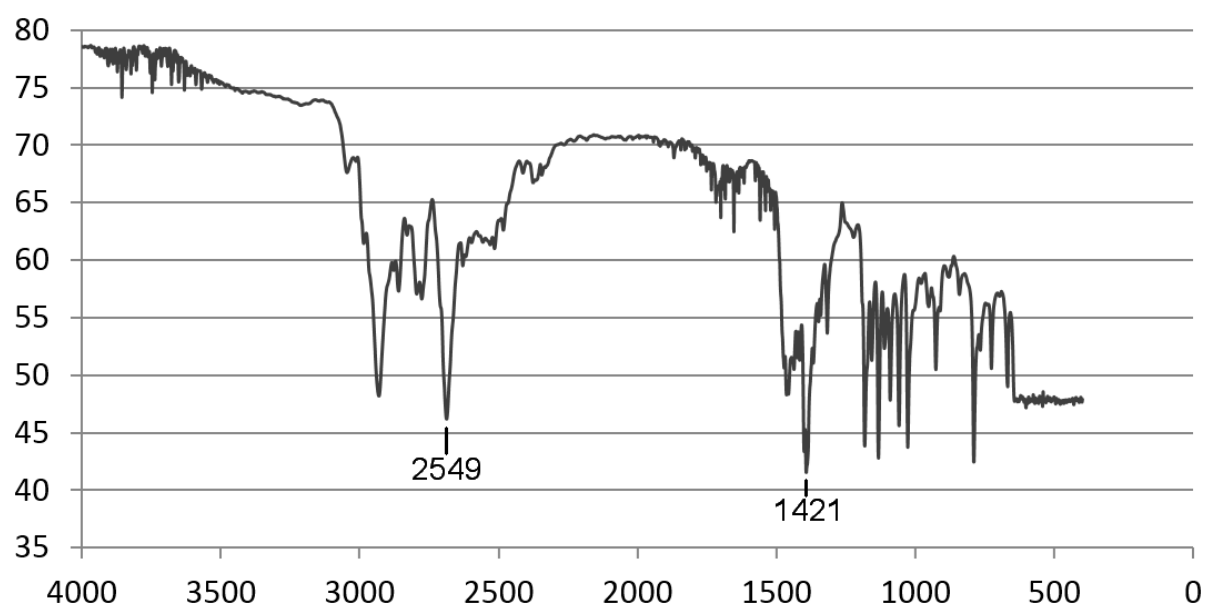


Figure S2. IR spectrum of compound 6

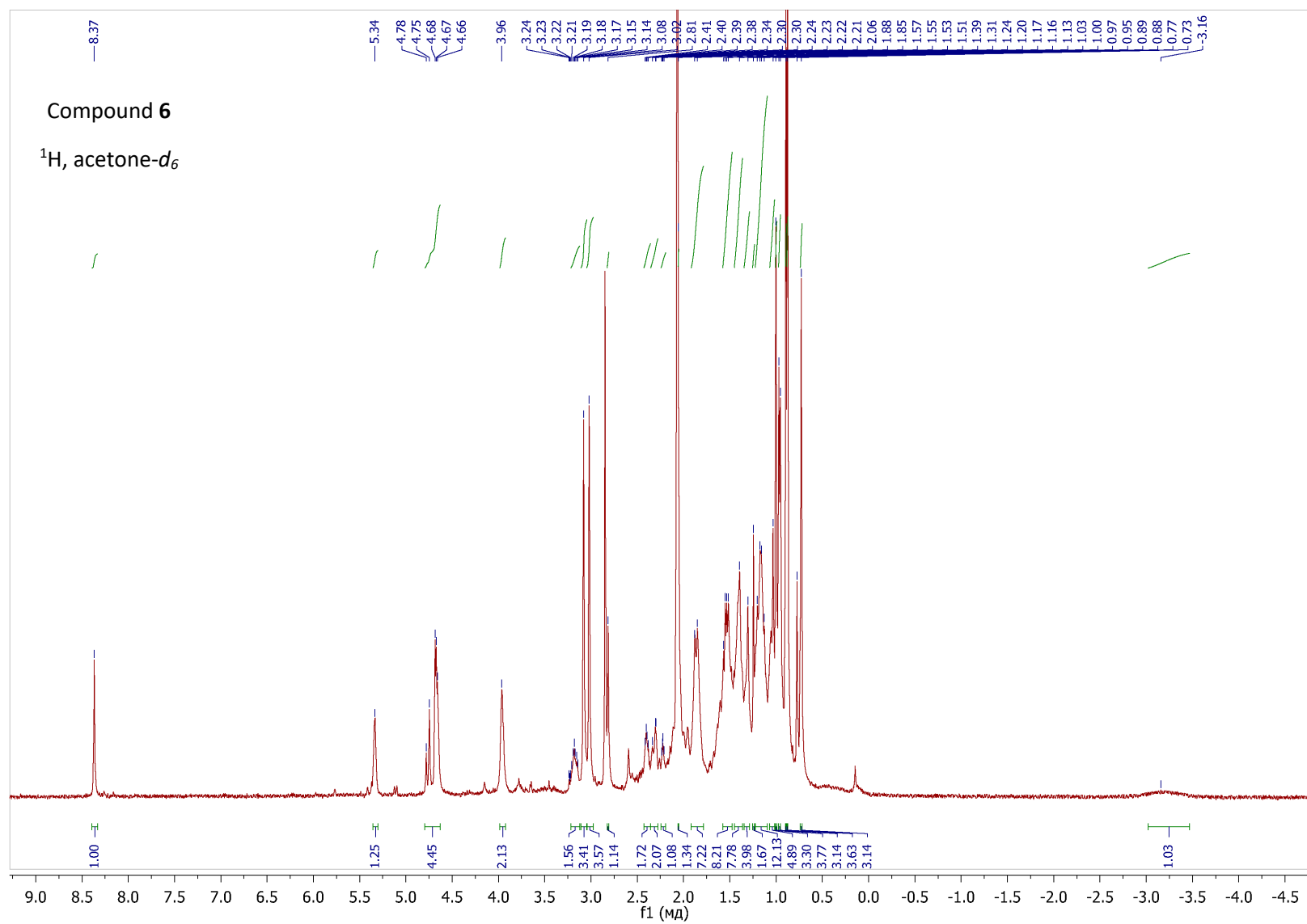


Figure S3. ^1H NMR spectrum of compound **6**

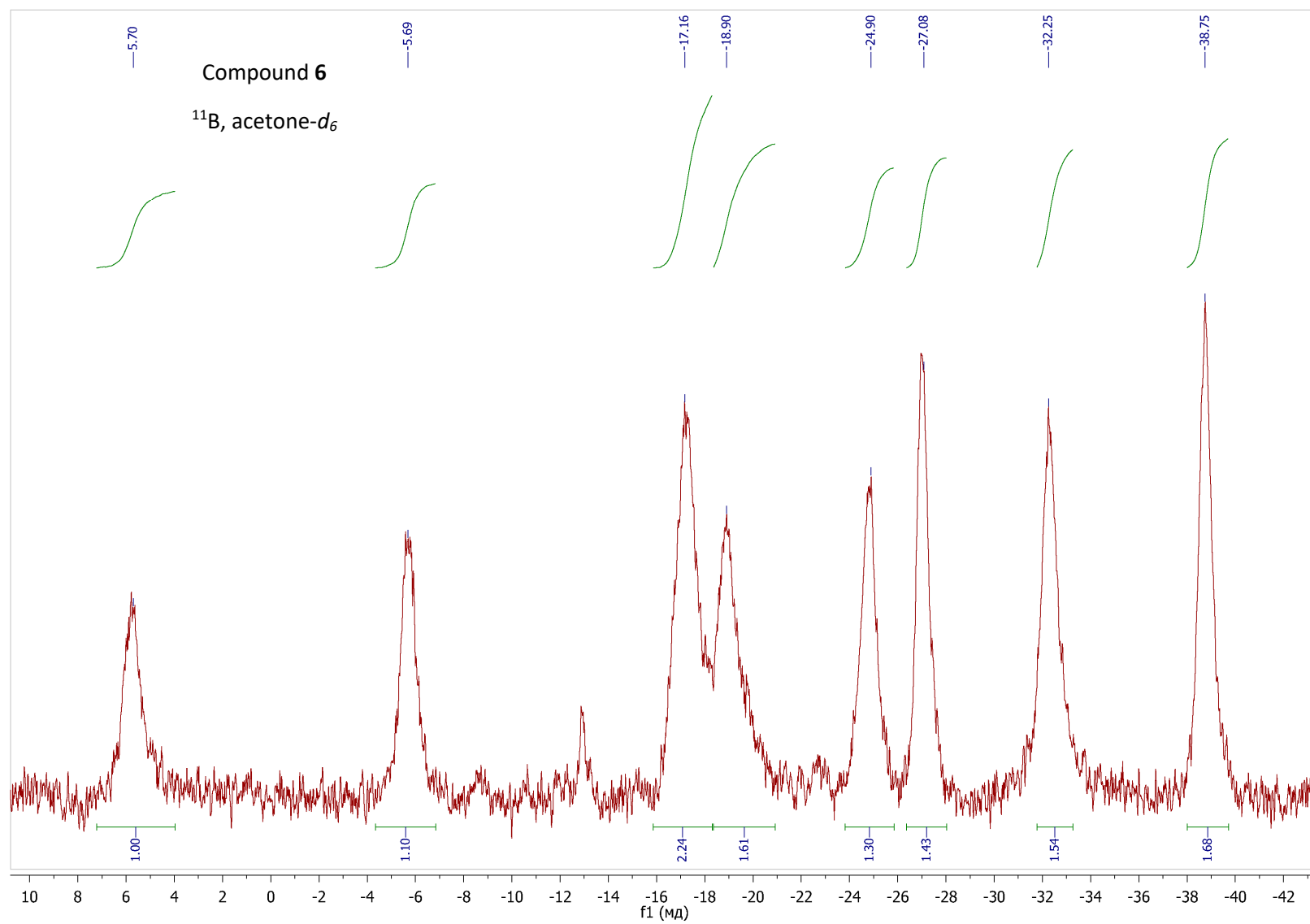


Figure S4. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **6**

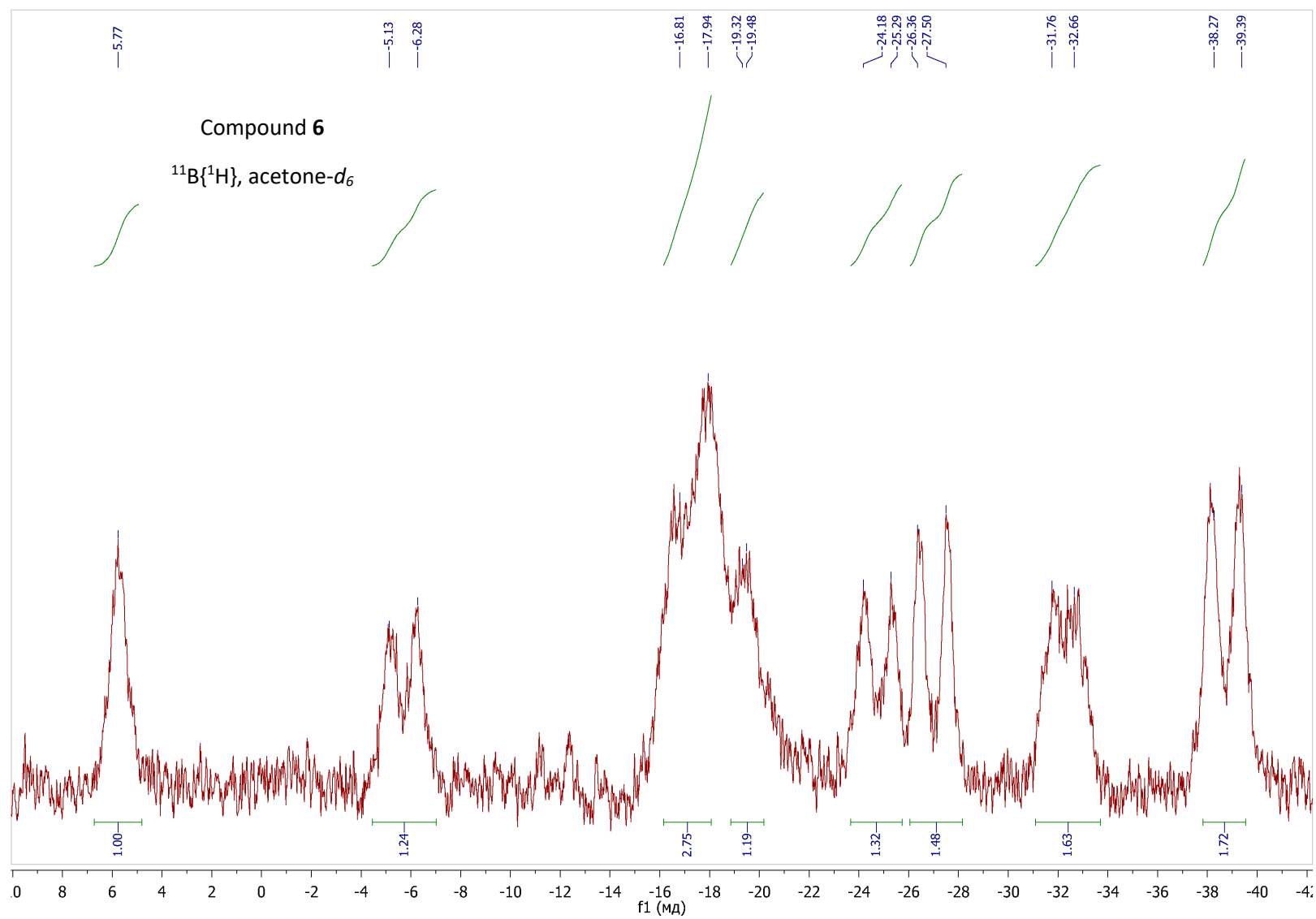


Figure S5. ^{11}B NMR spectrum of compound 6

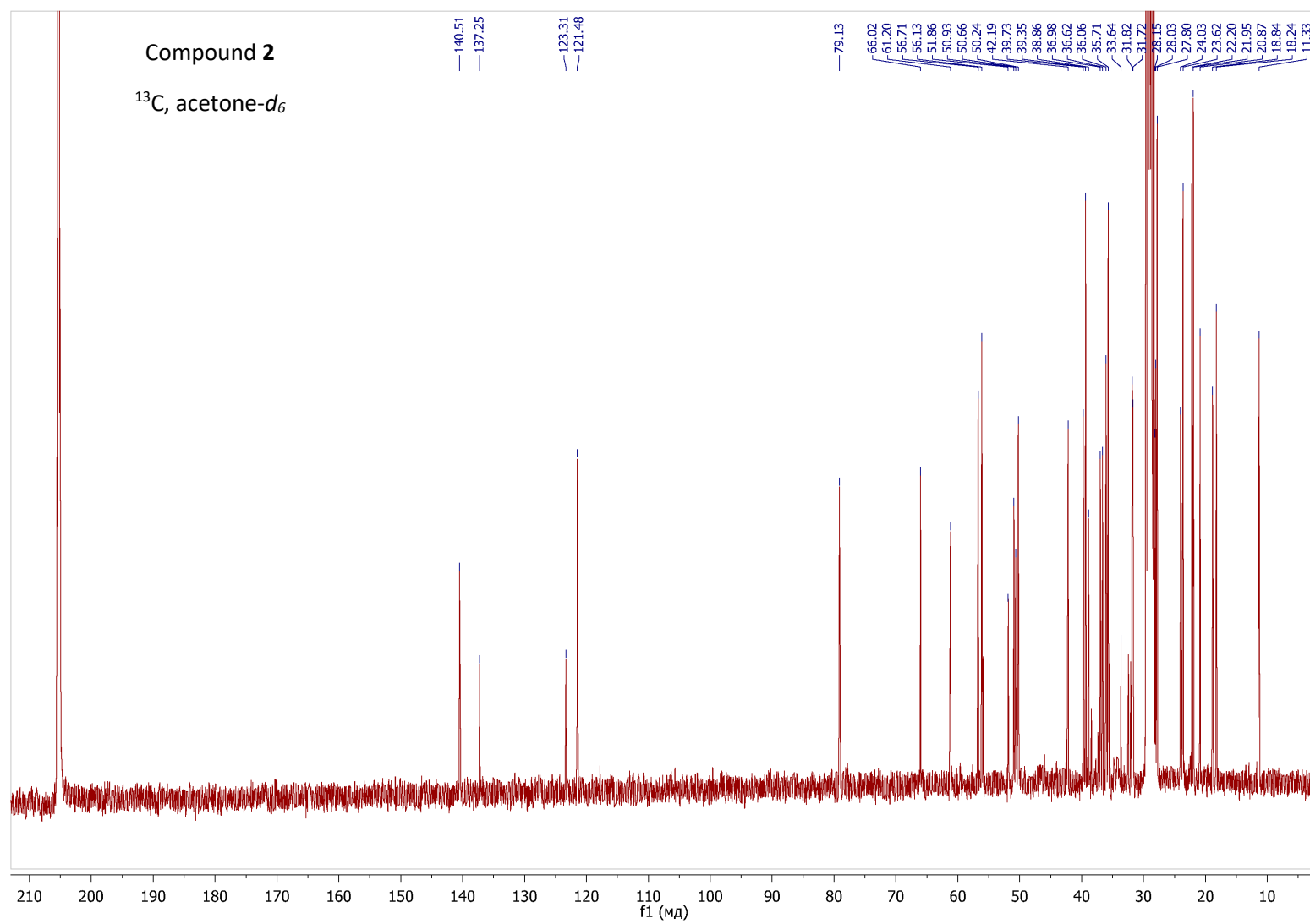


Figure S6. ^{13}C NMR spectrum of compound 6