Supplementary Material

3-(2-Nitrobenzyl)quinoxalin-2-ones, and pyrido- and 1,2,5-oxadiazolo-fused 2-(2-nitrobenzyl)pyrazin-3-ones in the synthesis of bi-, bis- and condensed heterocyclic systems

Vera L. Mamedova,[a] Victor V. Syakaev,[a] Il'dar Kh. Rizvanov,[a] Essam M. Mahrous,[b] Gul'naz Z. Khikmatova,[a] Sevil V. Mamedova,[b] Leisan R. Shamsutdinova,[a] Elena L. Gavrilova,[b] and Vakhid A. Mamedov*[a]

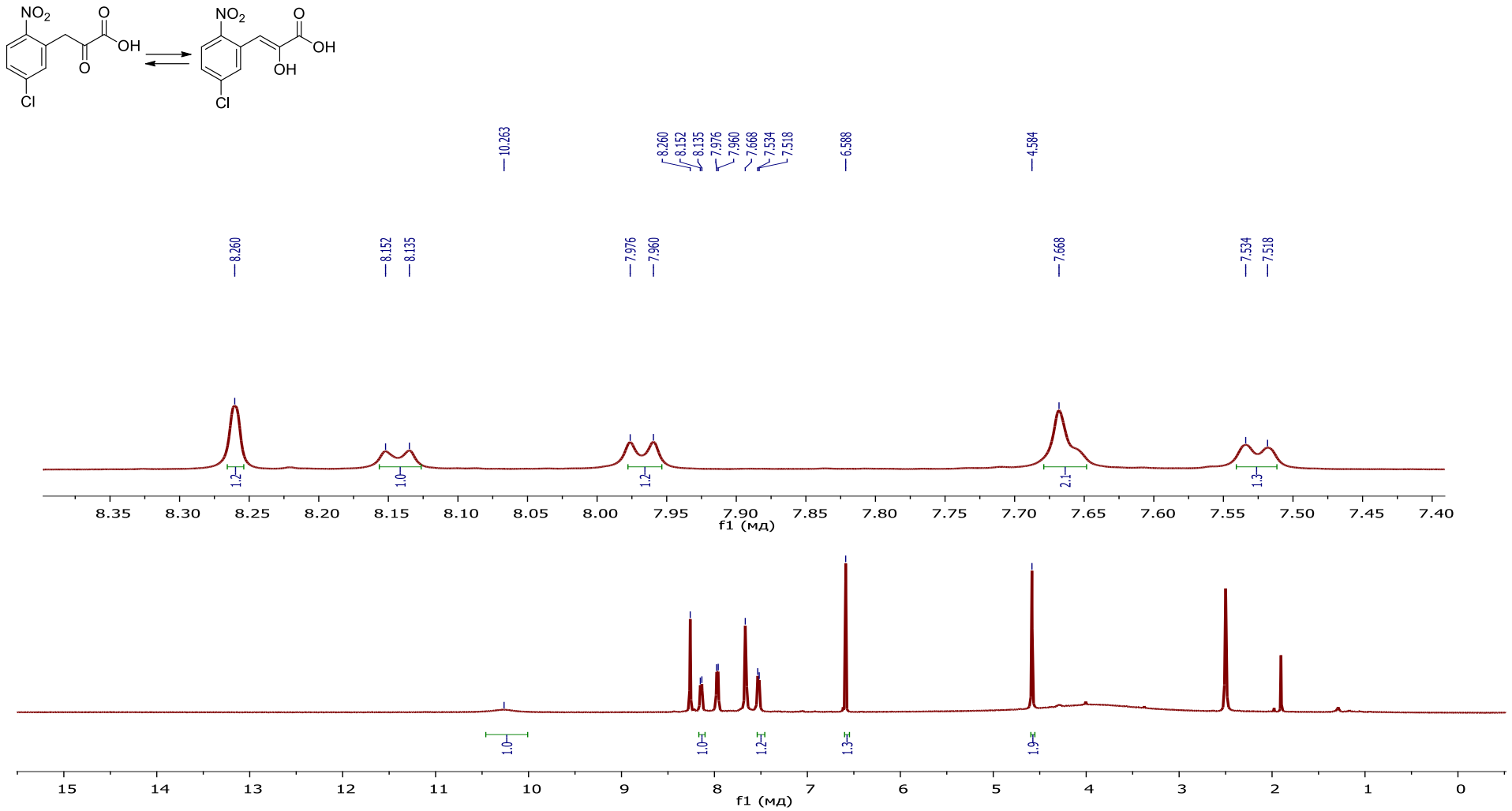
[a]*Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Arbuzov Str. 8, 420088 Kazan, Russian*

[b]*Kazan National Research Technological University, Karl Marx Str. 68, 420015 Kazan, Russian*

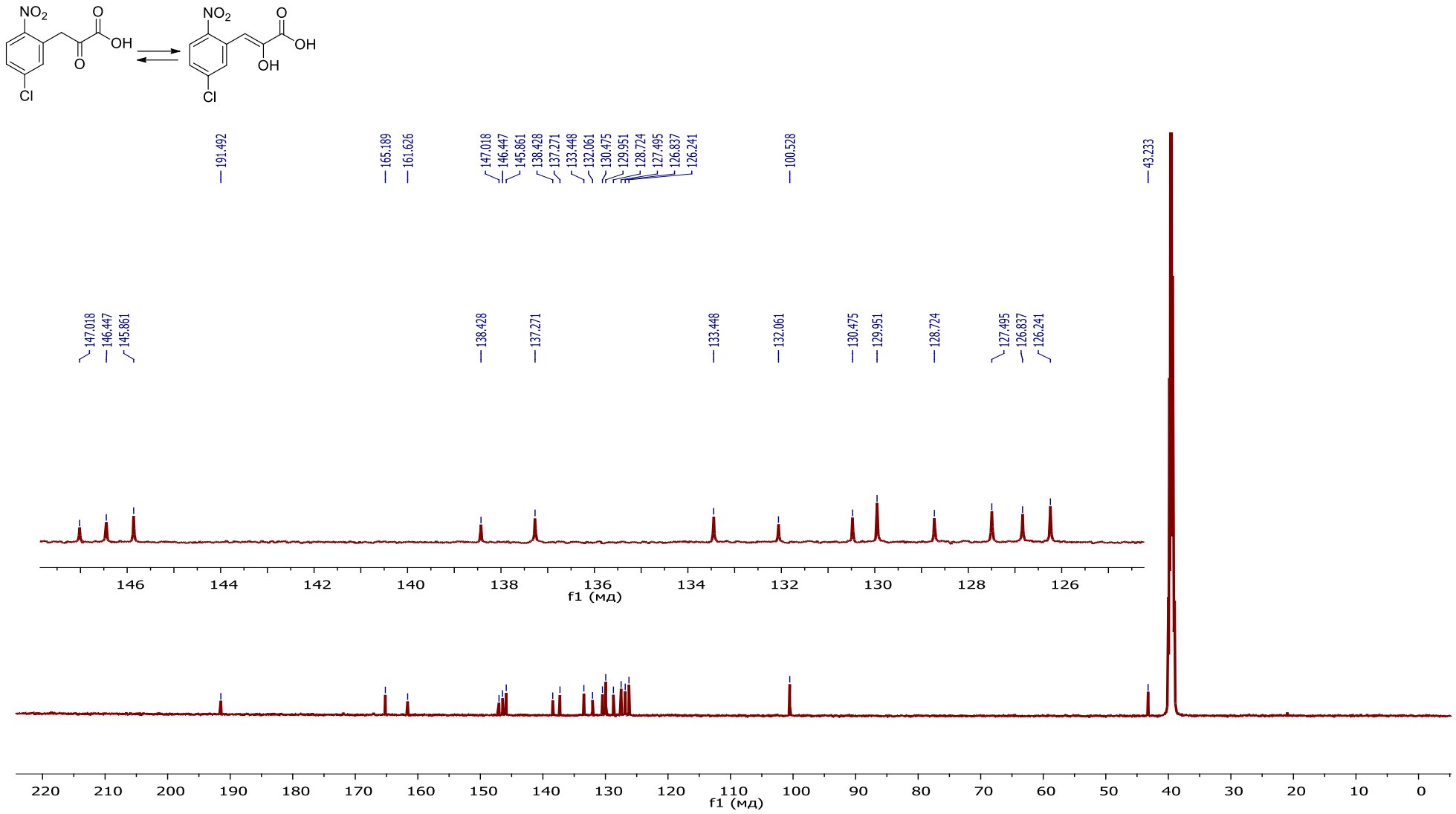
Email: mamedov@iopc.ru

Table of Contents

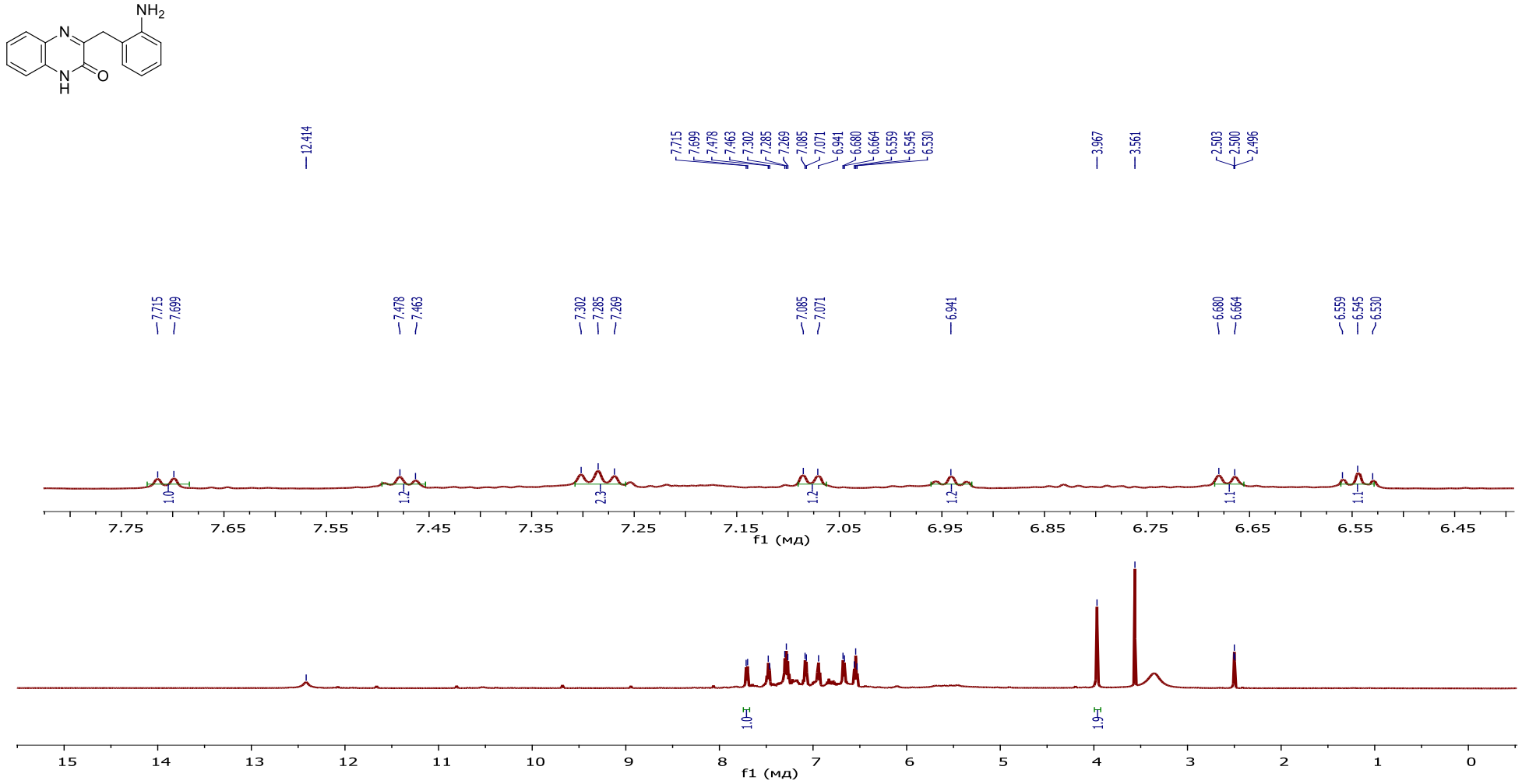
NMR Spectrum for 3-(2-nitro-5-chlorophenyl)pyruvic acid (**5**)_____S2
NMR Spectrum for 3-(2-aminobenzyl)quinoxalin-2(1*H*)-one (**6a**) _____S4
NMR Spectrum for 2-(1*H*-indol-2-yl)-1*H*-benzo[*d*]imidazoles (**7**) _____ S6
NMR Spectrum for 2-(2-nitrobenzyl)pyrido[2,3-*b*]pyrazin-3(4*H*)-one (**8**) _____S12
NMR Spectrum for (Z)-2-(2-nitrobenzyliden)-1,2-dihydro-1,2,5-oxadiazolo[3,4-*b*]pyrazin-3(4*H*)-one (**9**) _____ S14
NMR Spectrum for *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**) _____S16
NMR Spectrum for 4,11-dihydro-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-b]quinoline (**15**)_____S20
1D DPFGNOE Spectrum with selective excitation with mixing time of 600 ms of H6-Ar (b) and ^{1}H NMR spectrum (a) (DMSO, 303K) for (Z)-2-(2-nitrobenzylidene)-1,2-dihydro-1,2,5-oxadiazolo[3,4-*b*]pyrazin-3(4*H*)-one (**9**) _____S22
MS (MALDI) For *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**) _____S23
MS (ESI-QTOF) for 4,11-dihydro-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-b]quinoline (**15**) _____S24



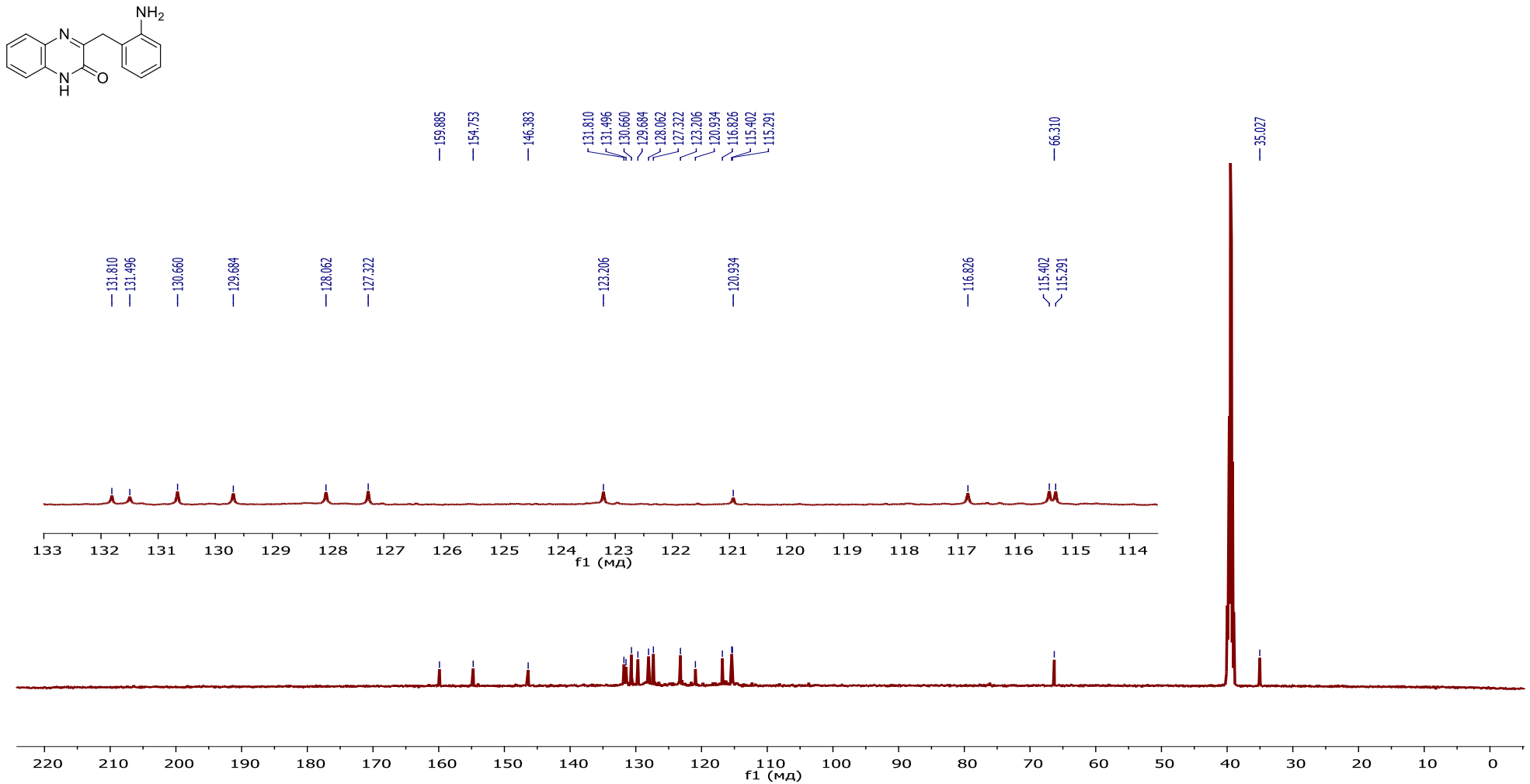
^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 3-(2-nitro-5-chlorophenyl)pyruvic acid (**5**)



^{13}C NMR Spectrum (126 MHz, DMSO, 303K) for 3-(2-nitro-5-chlorophenyl)pyruvic acid (**5**)



^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 3-(2-aminobenzyl)quinoxalin-2(1*H*)-one (**6a**)



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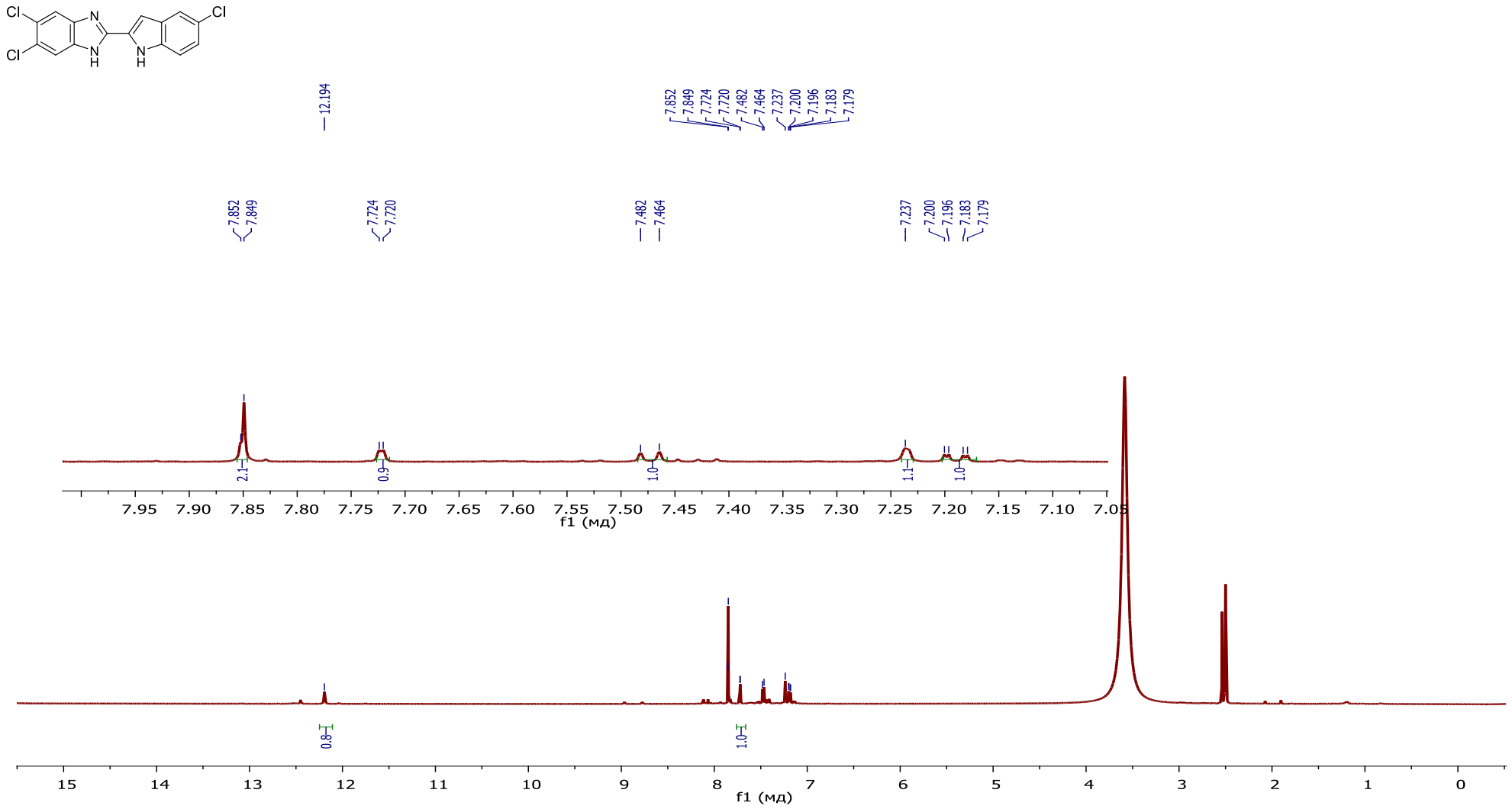
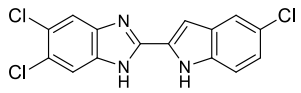
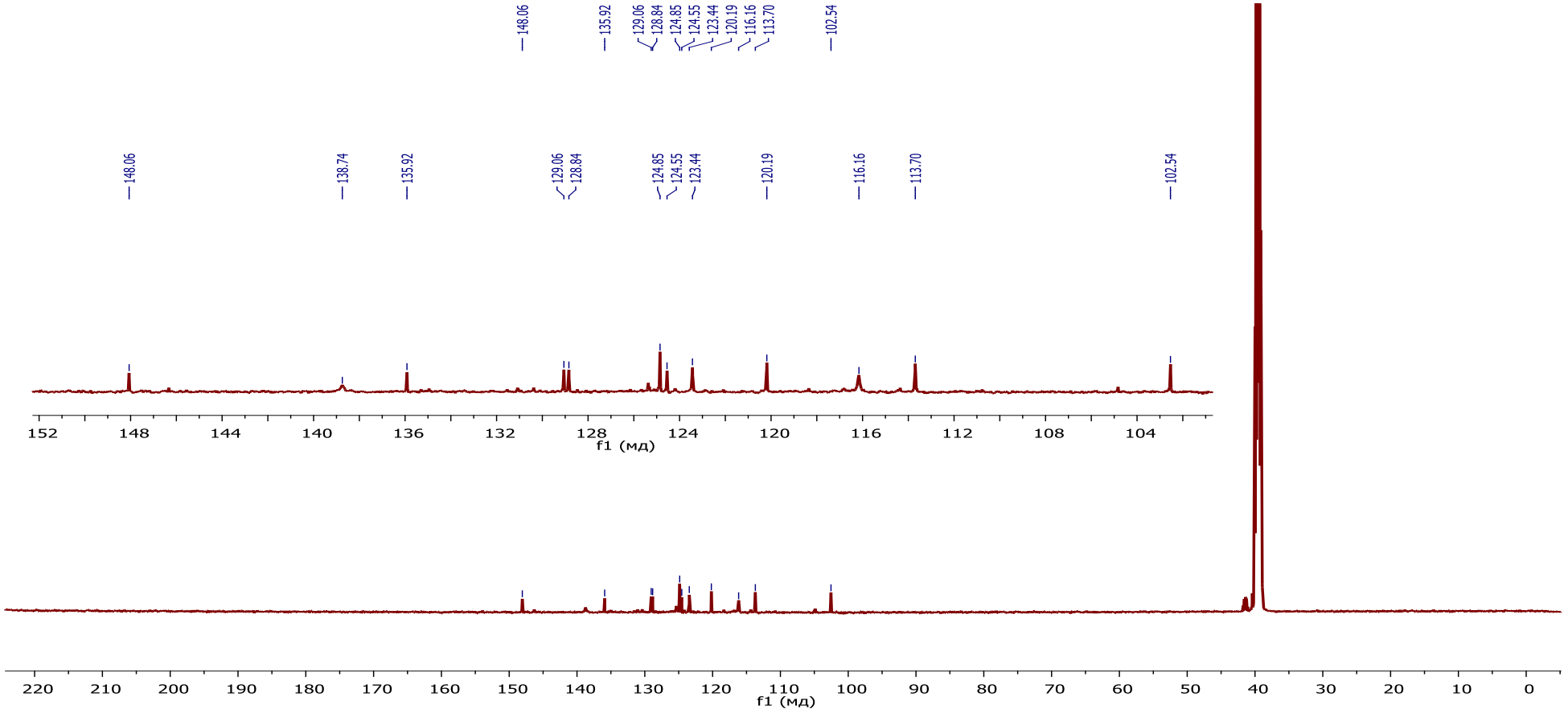


^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 5,6-dichloro-2-(5-chloro-1*H*-indol-2-yl)-1*H*-benzo[*d*]imidazole (**7b**)





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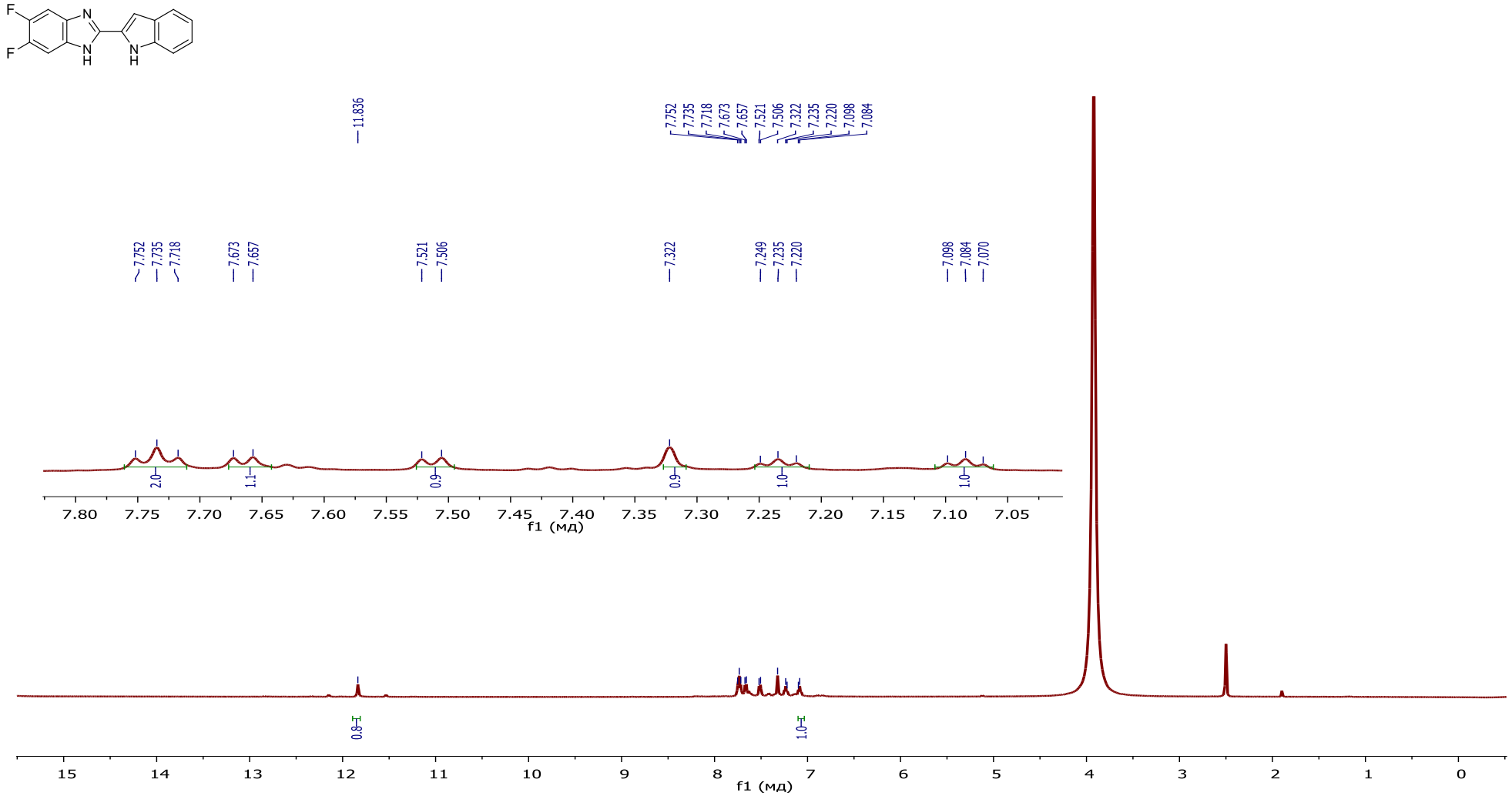
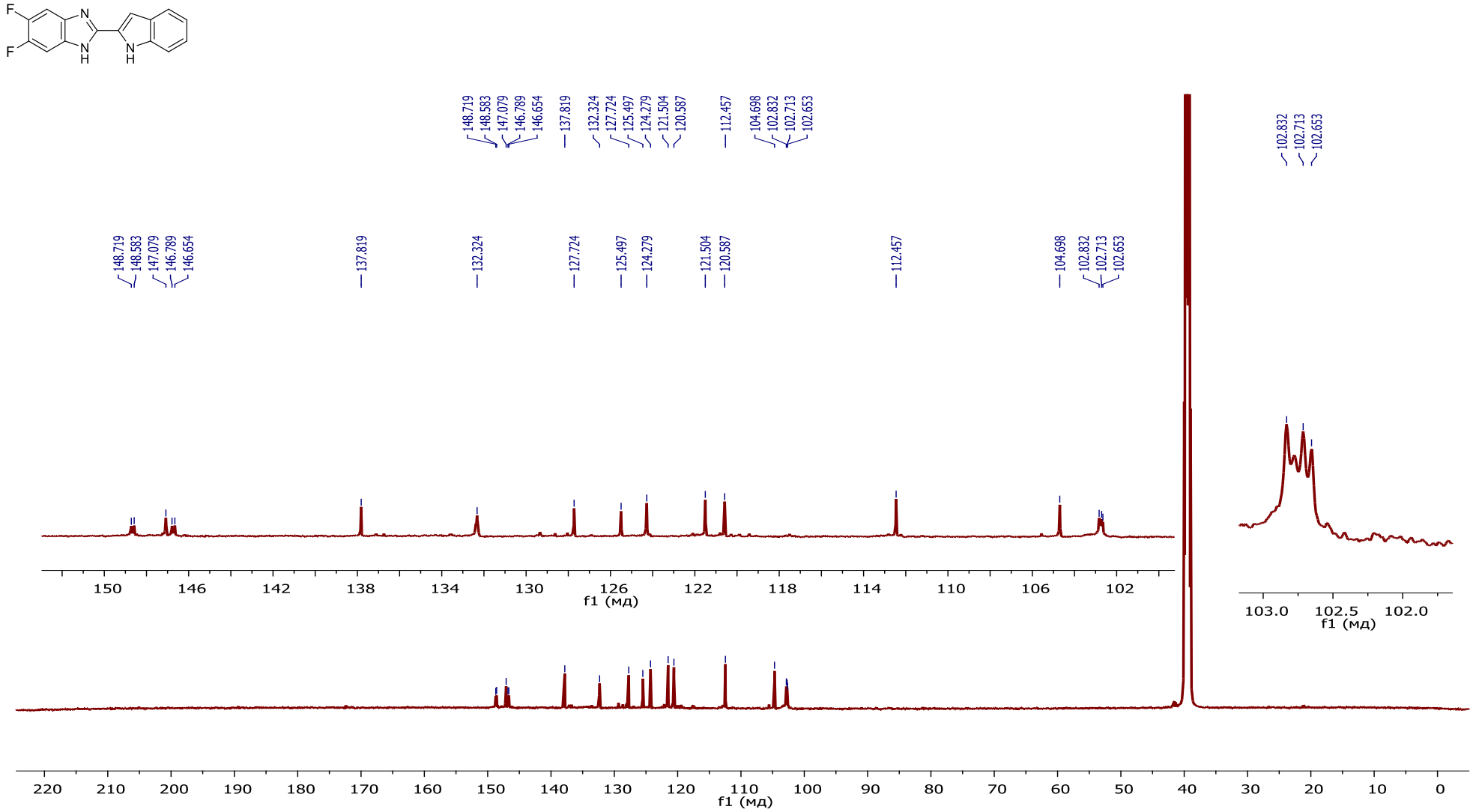


^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 5,6-difluoro-(1*H*-indol-2-yl)-1*H*-benzo[*d*]imidazole (**7c**)



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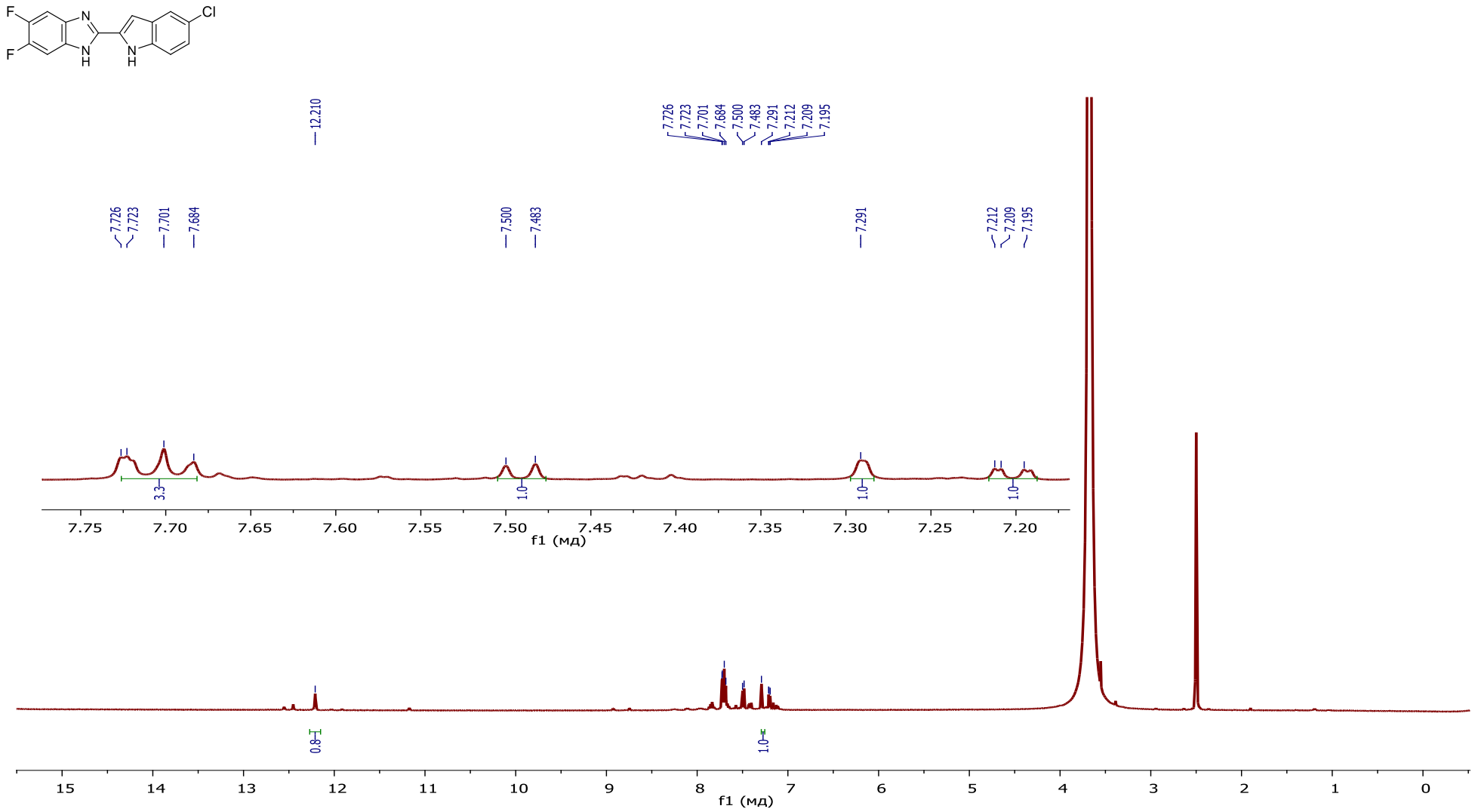
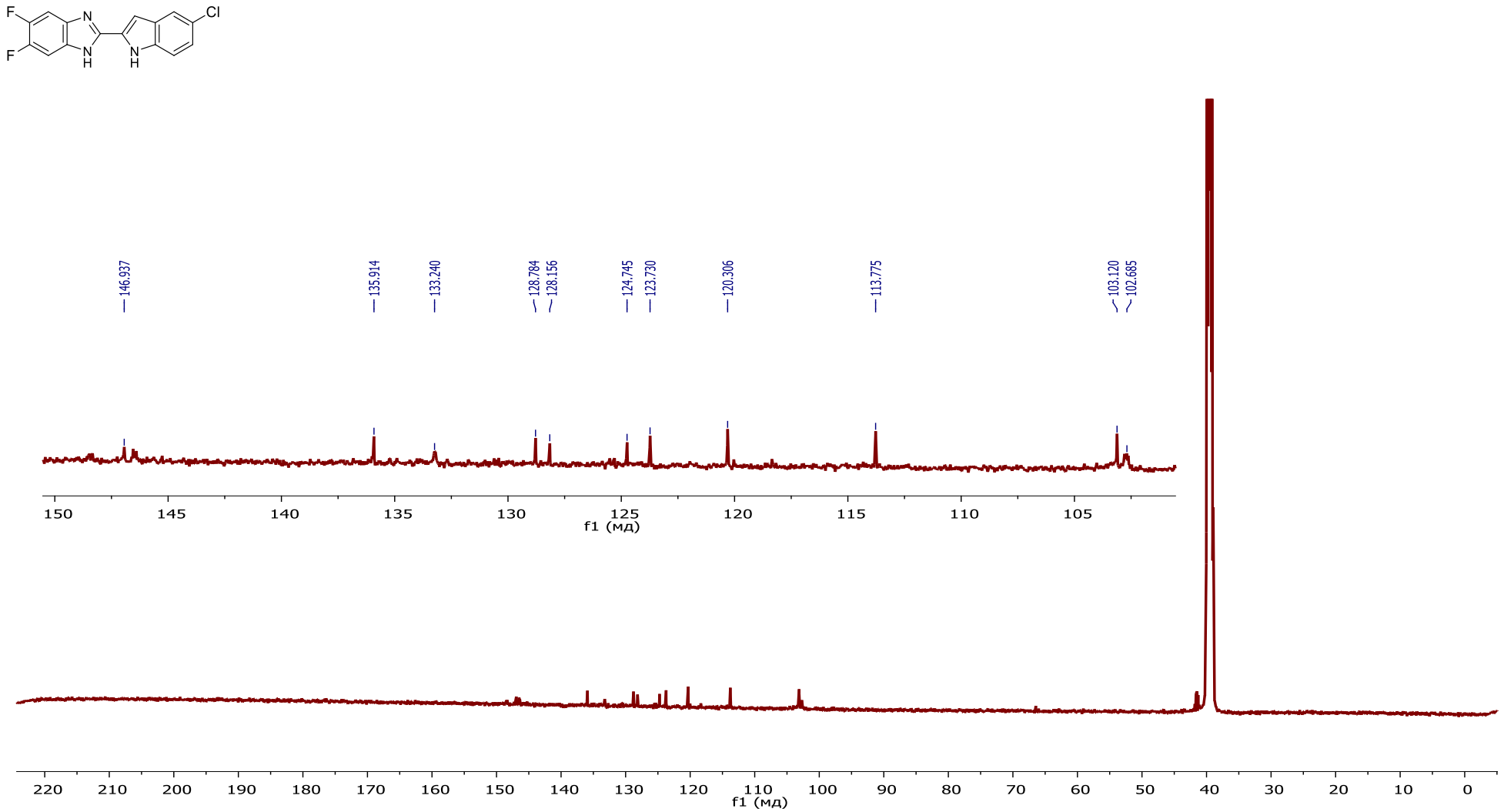


^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 5,6-difluoro-2-(5-chloro-1*H*-indol-2-yl)-1*H*-benzo[*d*]imidazole (**7d**)



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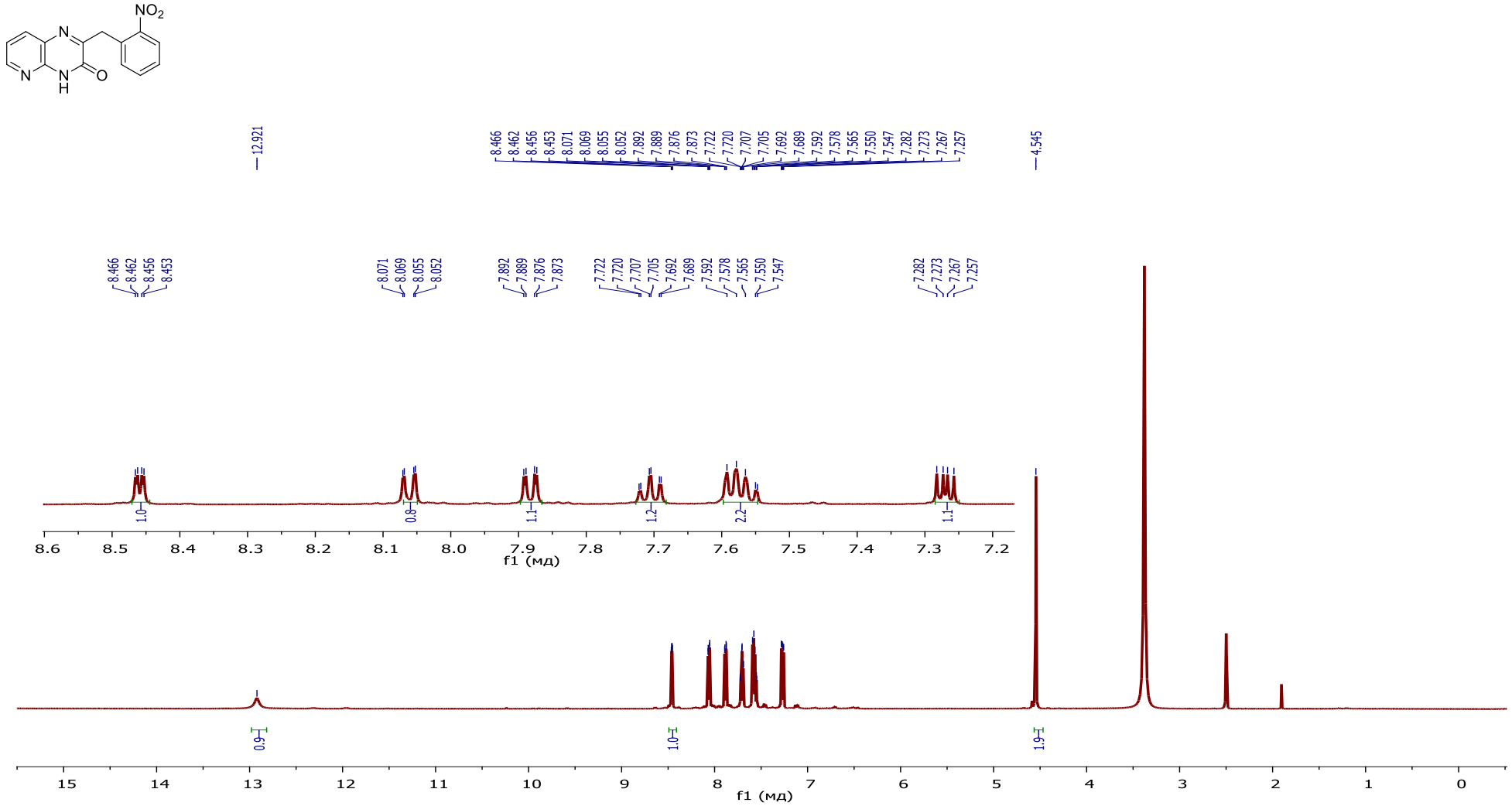
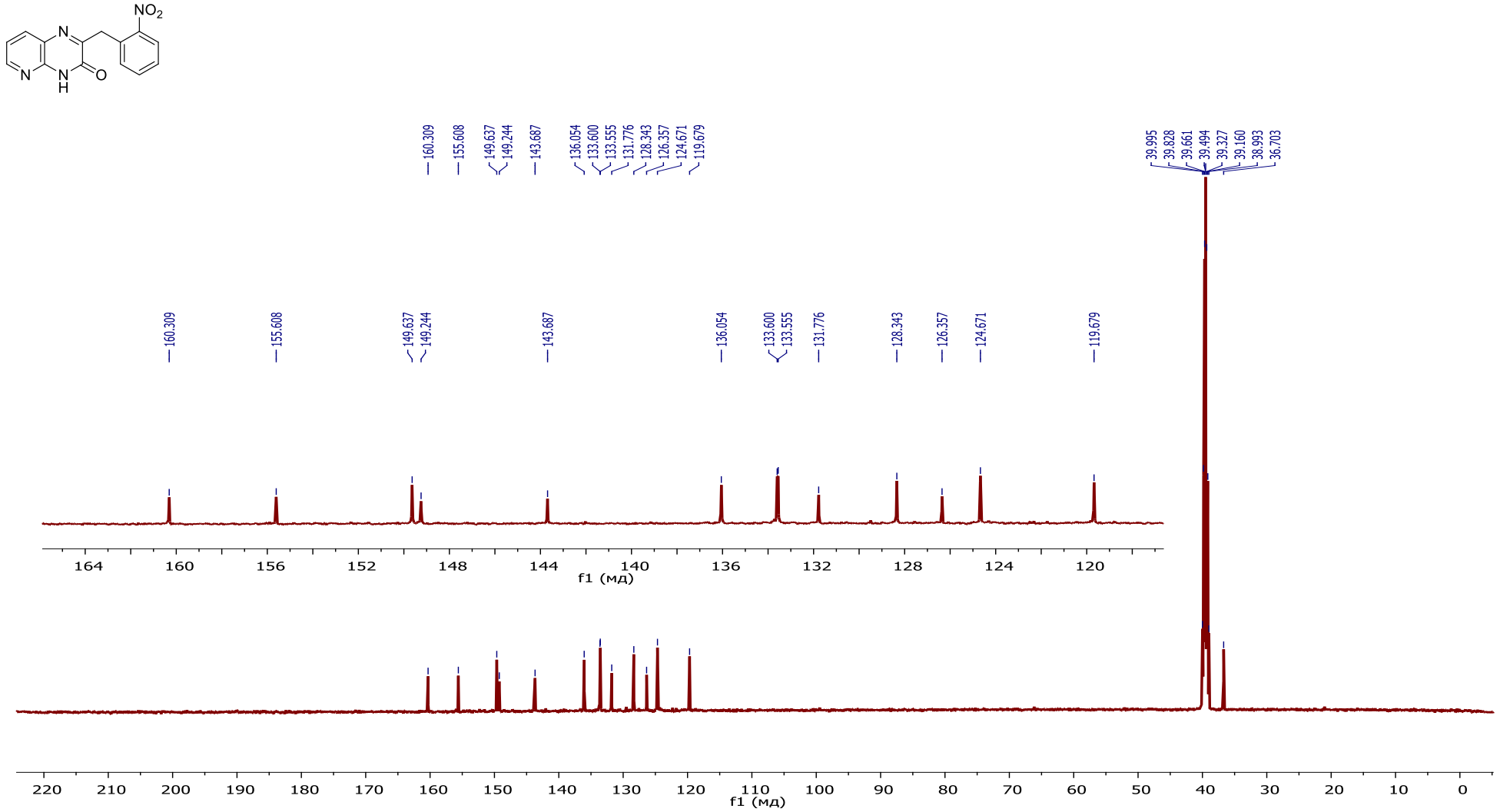


^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for 2-(2-nitrobenzyl)pyrido[2,3-*b*]pyrazin-3(4*H*)-one (**8**)



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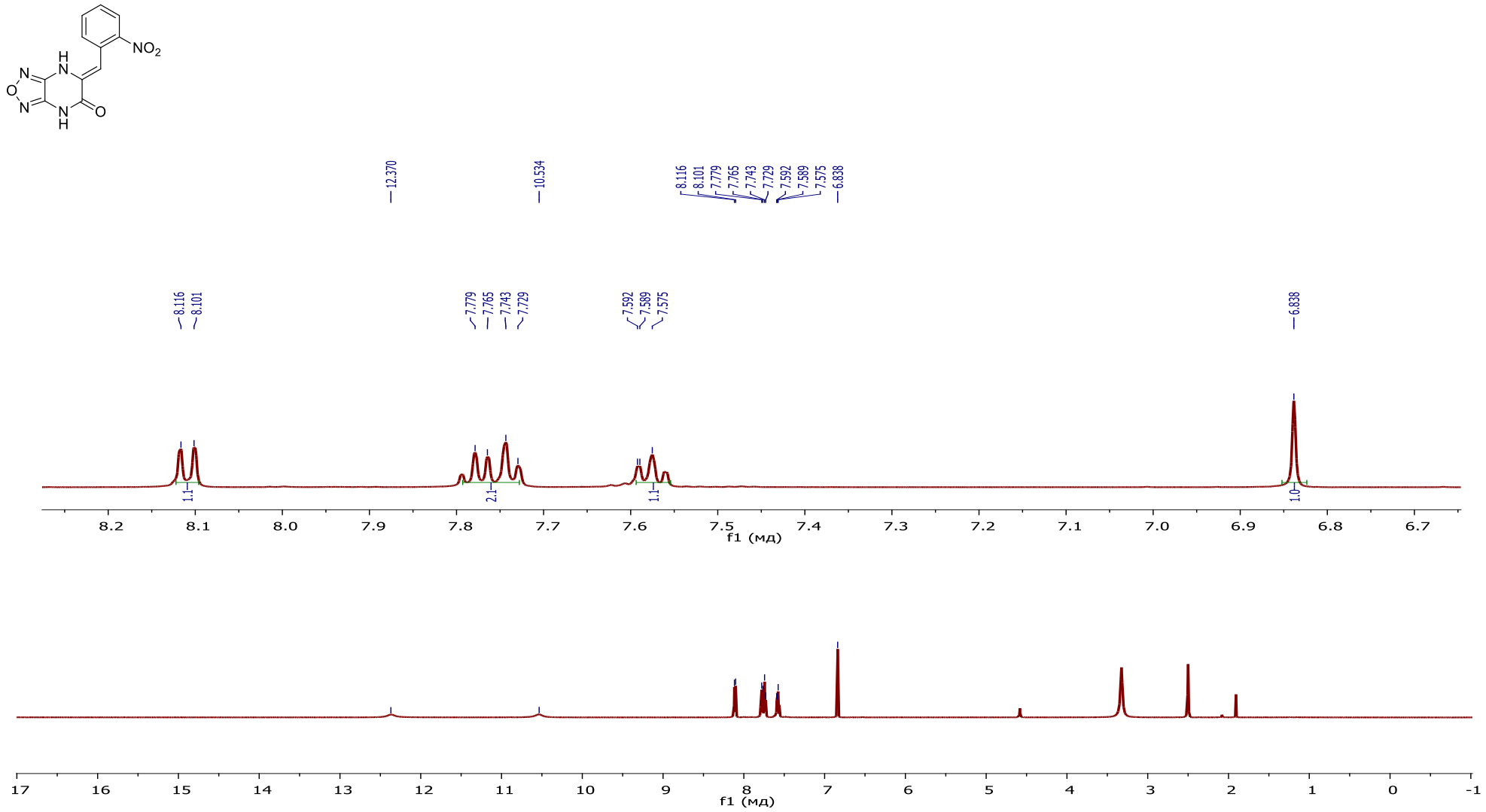

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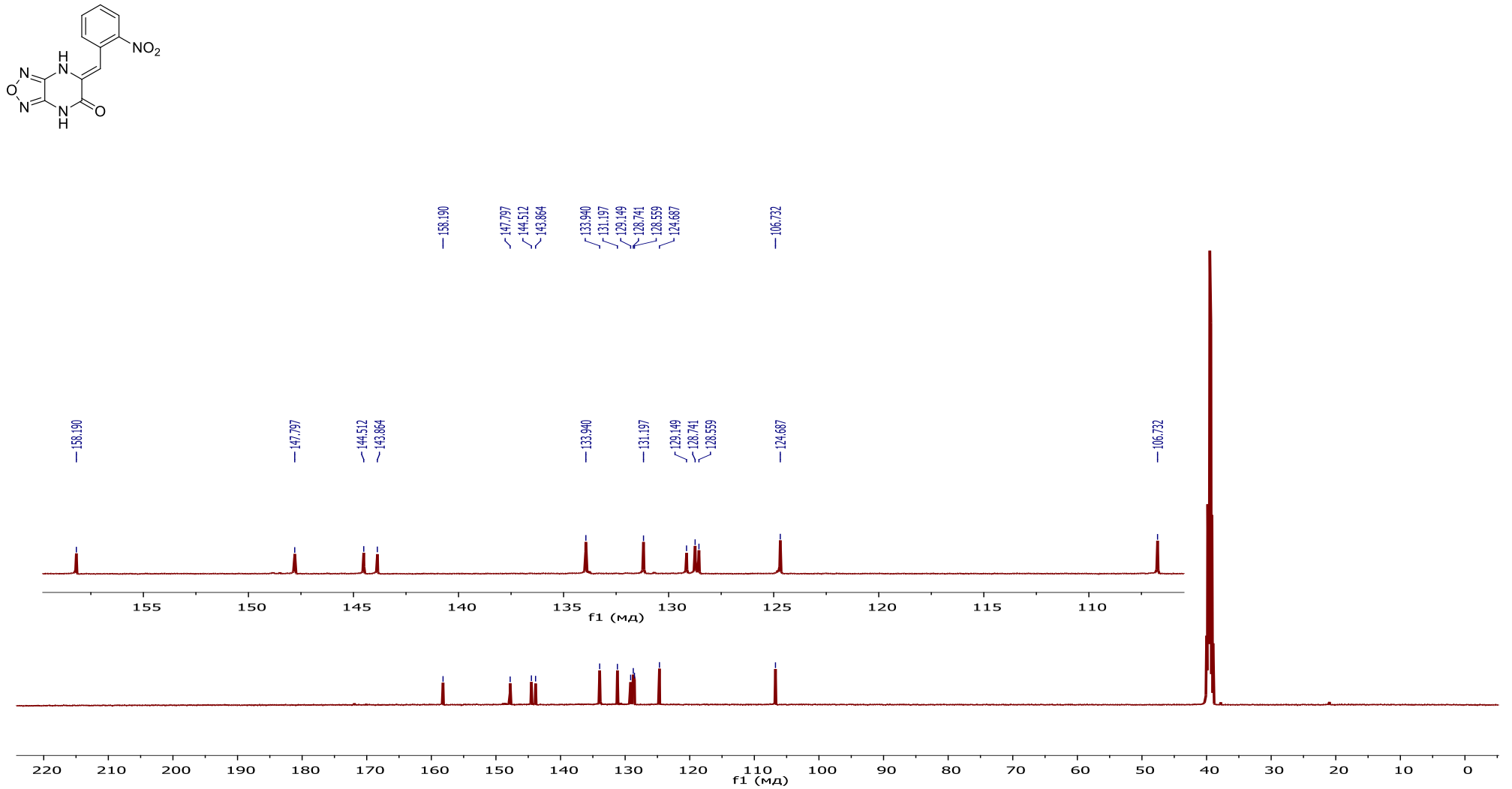

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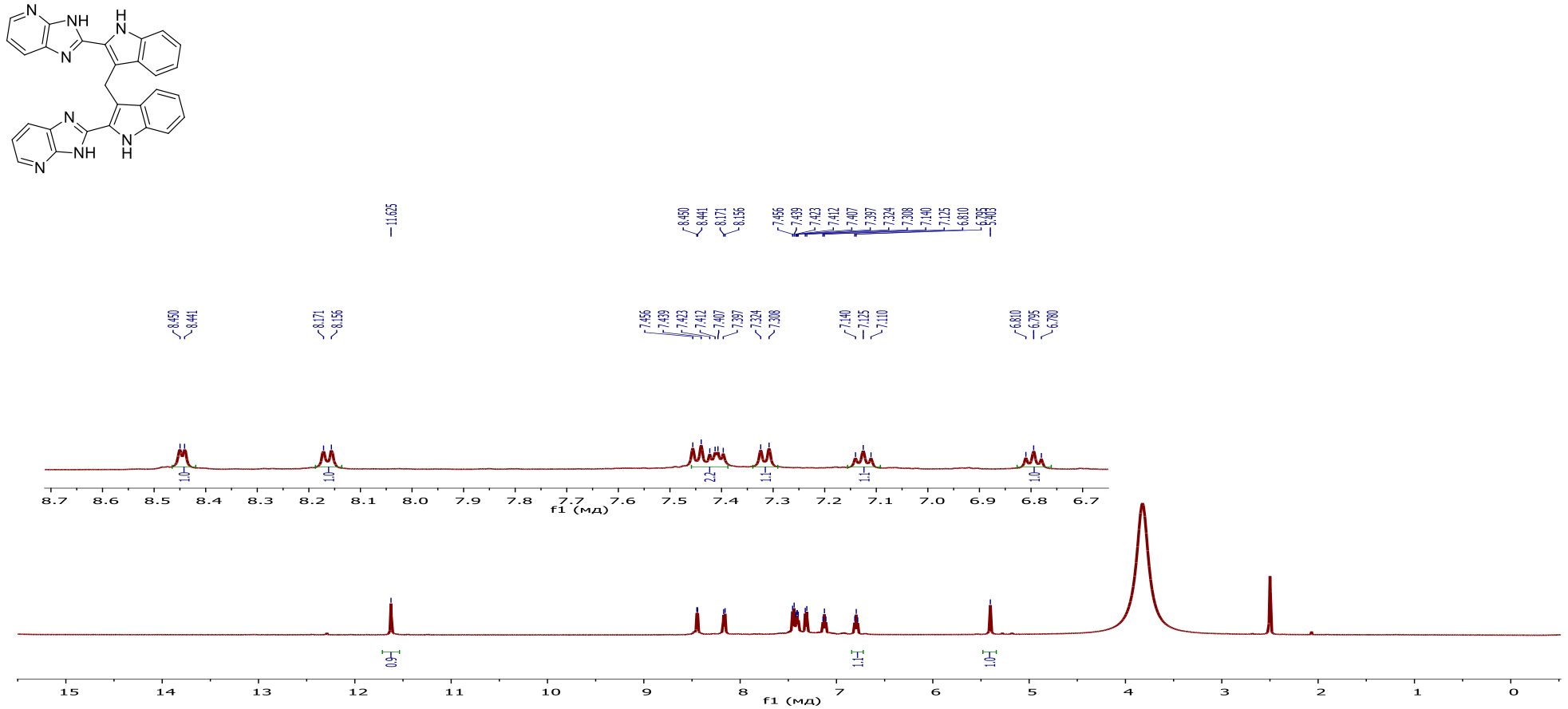
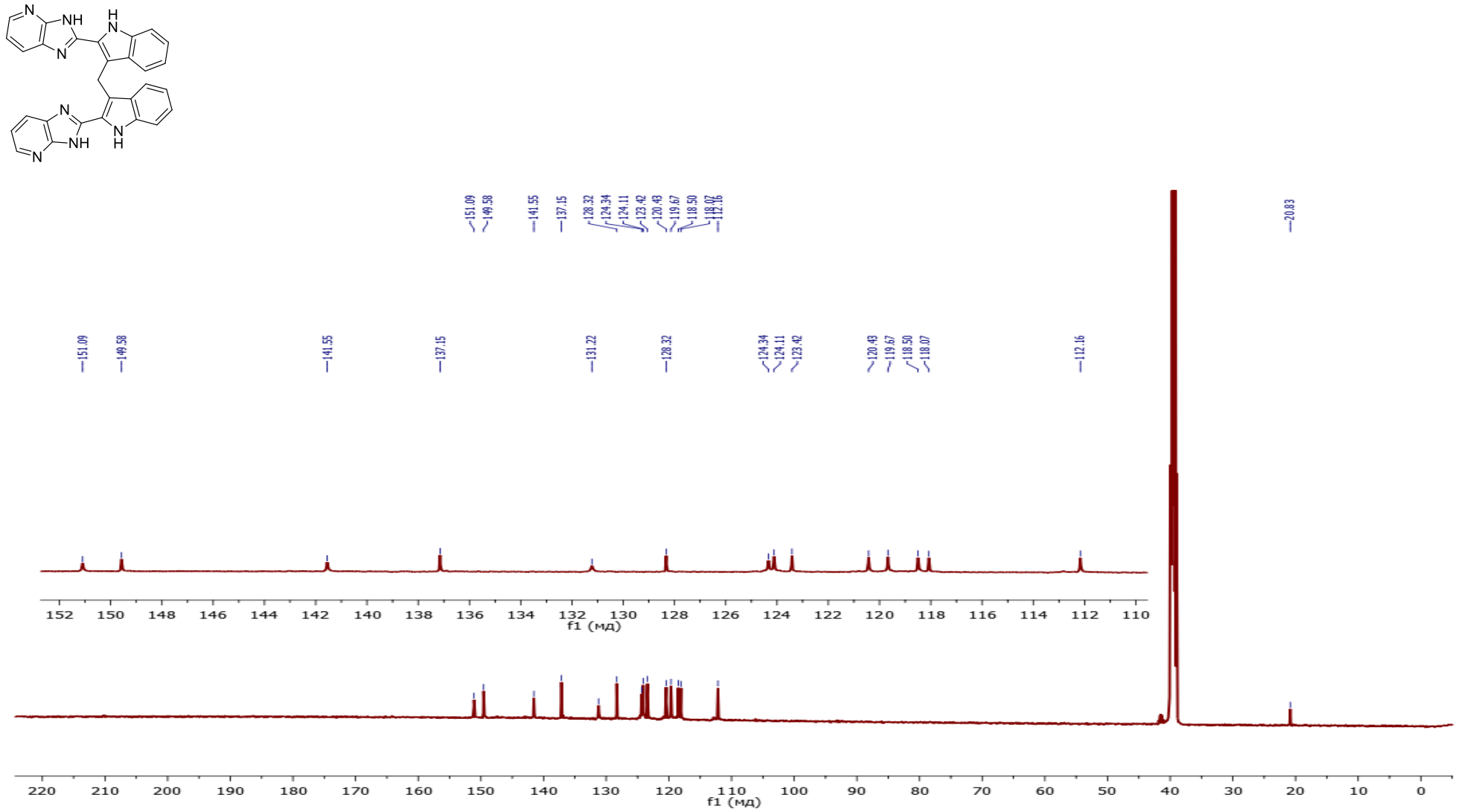
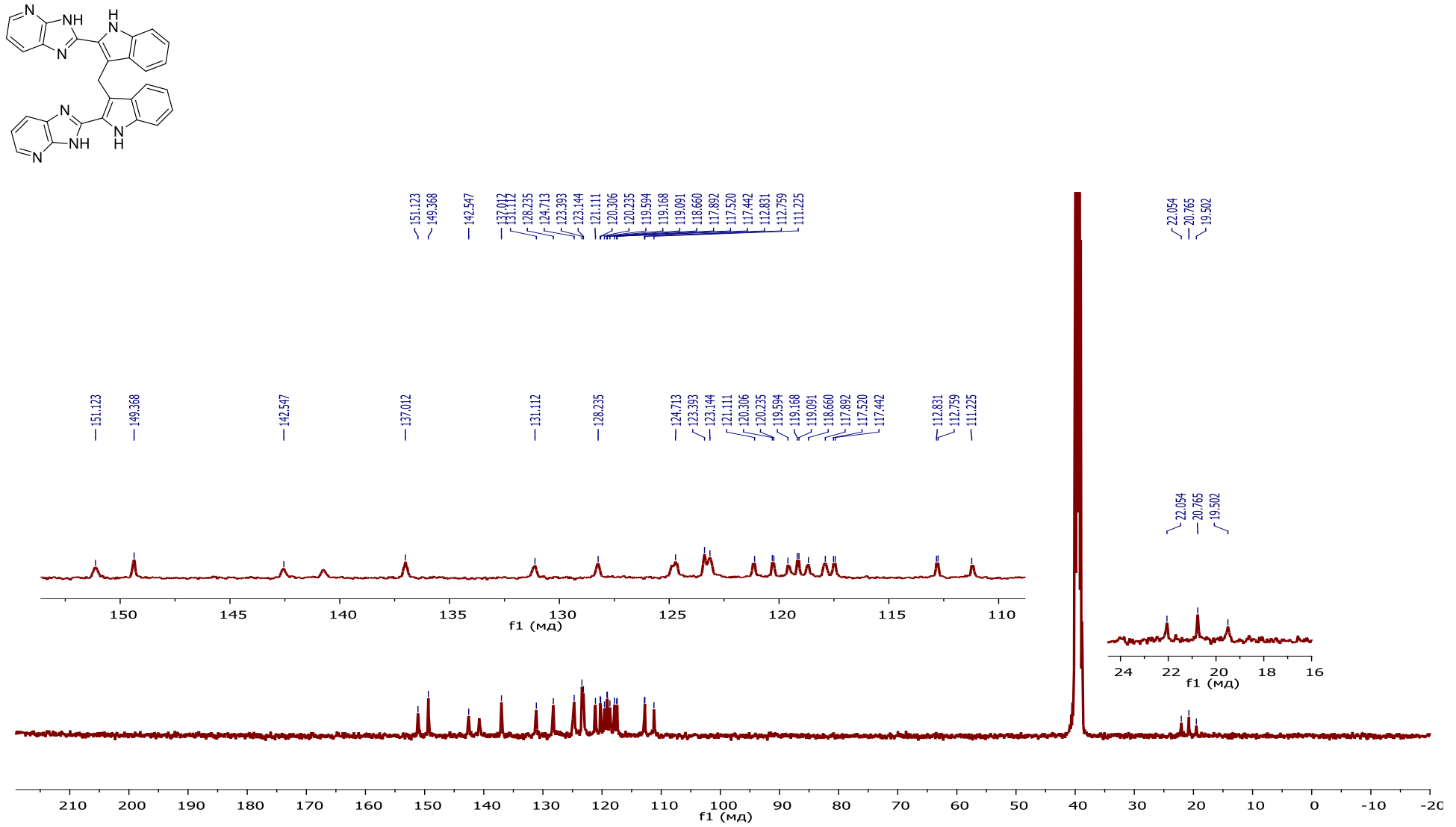


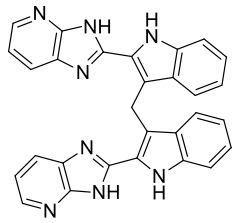
^{1}H NMR Spectrum (500 MHz, DMSO, 303K) for *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**)

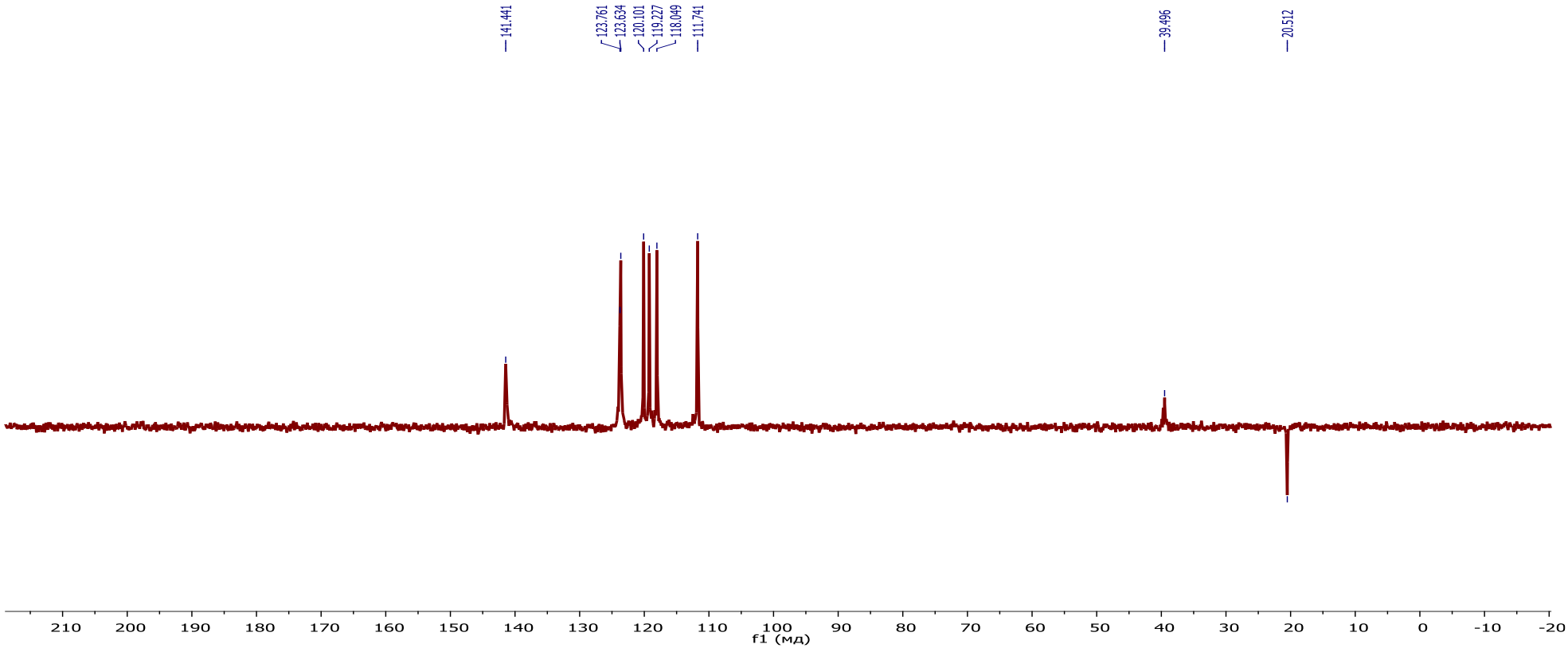


^{13}C NMR Spectrum (126 MHz, DMSO, 303K) for *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**)

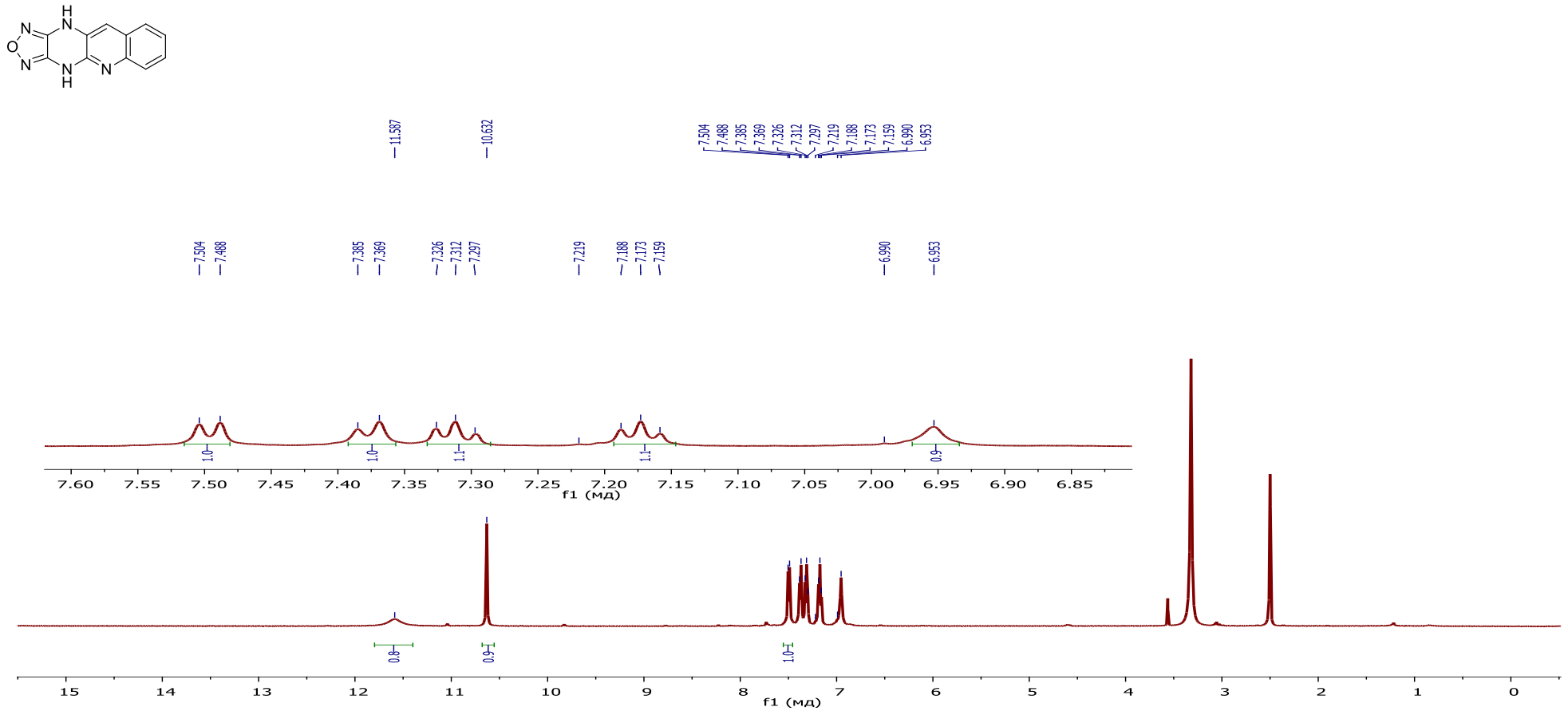


^{13}C DO NMR Spectrum (126 MHz, DMSO, 303K) for *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**)





^{13}C DEPT NMR Spectrum (126 MHz, DMSO, 303K) for *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**)



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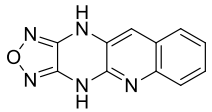
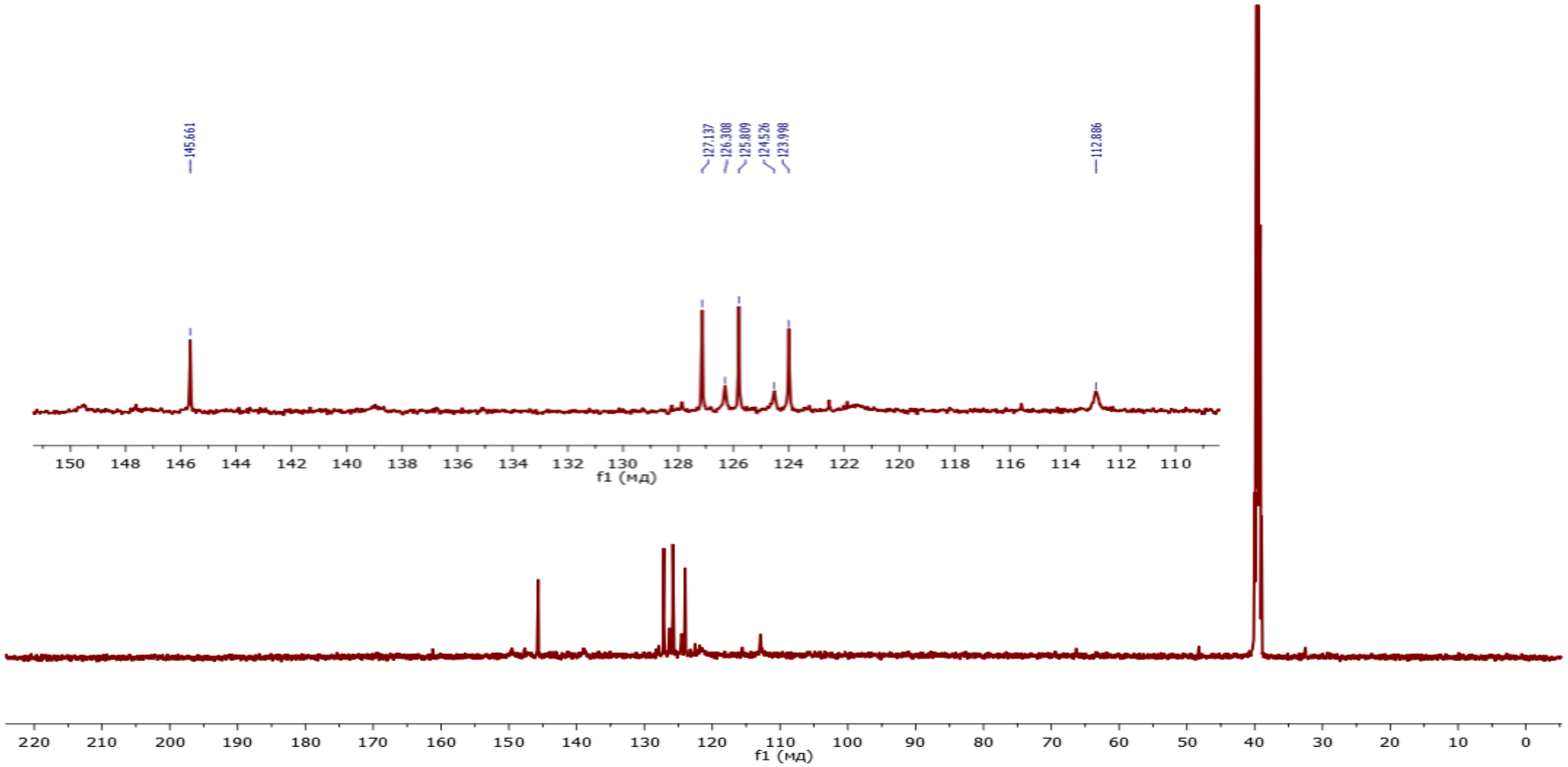
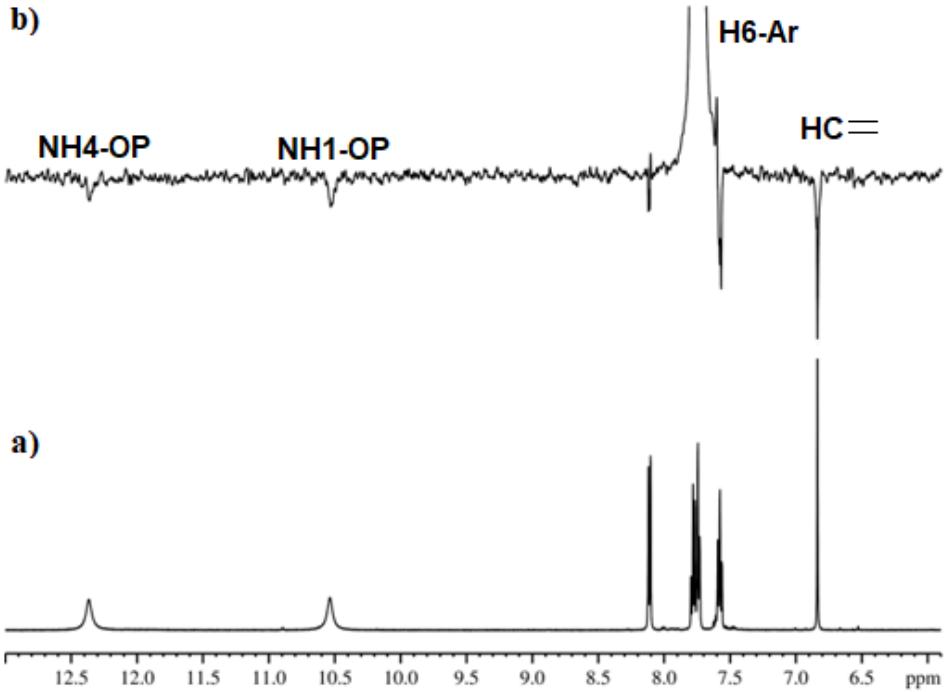
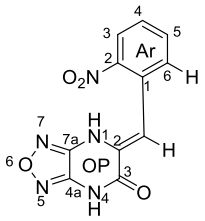




^{13}C NMR Spectrum (126 MHz, DMSO, 303K) for 4,11-dihydro-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-b]quinoline (**15**)

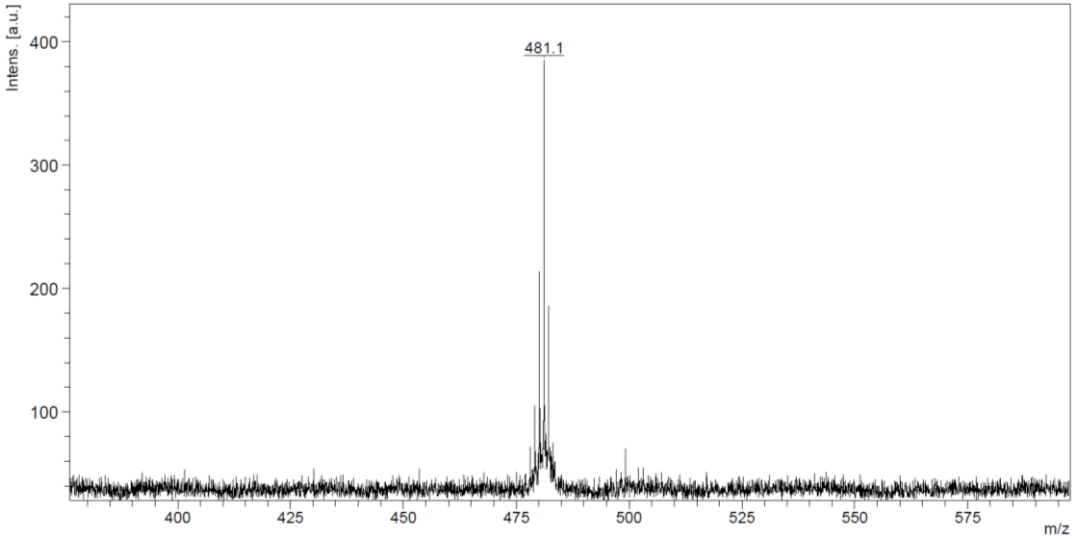


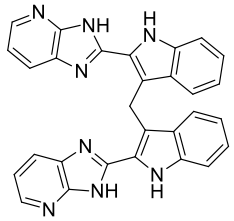


1D DPFGNOE Spectrum with selective excitation with mixing time of 600 ms of H6-Ar (b) and ^{1}H NMR spectrum (a) (DMSO, 303 K) for (Z)-2-(2-nitrobenzylidene)-1,2-dihydro-1,2,5-oxadiazolo[3,4-*b*]pyrazin-3(4*H*)-one (**9**).

The MALDI mass-spectra for **10** was obtained on an UltraFlex III TOF-TOF instrument in positive mode. The device is equipped with a solid-state laser Nd:YAG laser (λ = 355 nm, repetition rate 66.7 Hz). Measurements were made in the range m/z 200-2000. A mixture of the sample (2 mg/mL, DMSO) was prepared to determine the mass values. para-Nitroaniline (10 mg/mL, CH_3CN) was used as a matrix. Portions (0.5 µL) of the matrix solution and the analyzed mixture were sequentially applied to the target and evaporated. The metal target MTP AnchorChipTM was used. The m/z values of monoisotopic ions are given in the descriptions. The data was obtained using the FlexControl program (Bruker Daltonik GmbH, Germany) and processed using the FlexAnalysis 3.0 program (Bruker Daltonik GmbH, Germany).

Mass spectra (MALDI)

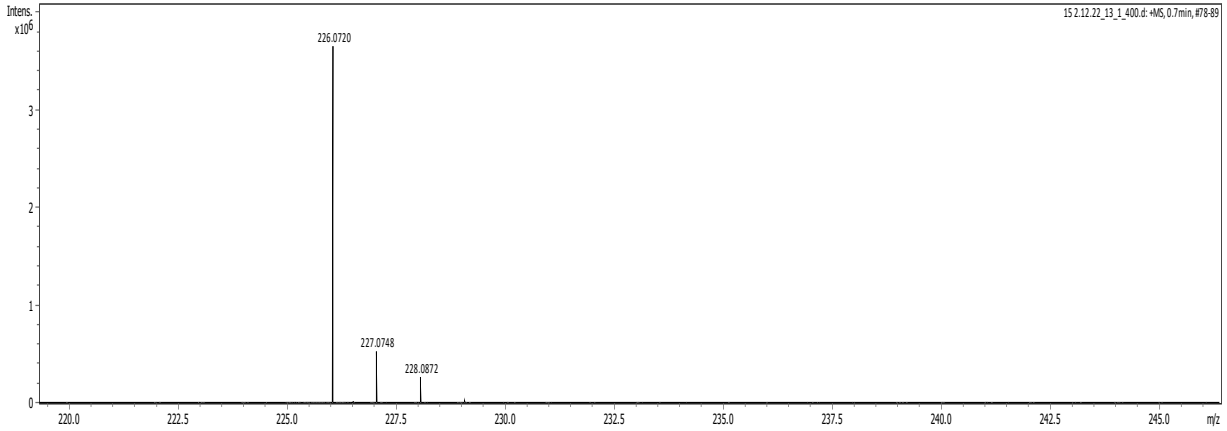




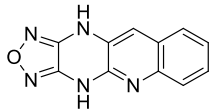
Molecular Weight: 480,52

Figure 1. MS (MALDI) For *bis*(2-(3*H*-imidazo[4,5-*b*]pyridin-2-yl)-1*H*-indol-3-yl)methane (**10**), m/z: $[M + H]^+$ 481

The high resolution mass spectra (HRMS) of **15** was obtained on an Impact II ESI-QTOF (Bruker Daltonic GmbH, Germany) mass spectrometer. Measurement was made in the range m/z 50-1900. The instrument was calibrated with Sodium formate. The sample was dissolved in DMF and redissolved in acetonitrile/water solution (70:30). An acetonitrile/water solution was used at a flow rate of 0.3 mL/min by binary pump. The specified composition allowed to provide the relative error in determining the masses no more than 2.0 ppm.



MS (ESI-QTOF) For 4,11-dihydro-[1,2,5]oxadiazolo[3′,4′:5,6]pyrazino[2,3-*b*]quinoline (**15**), m/z: $[M+H]^+$ ($C_{11}H_8ON_5$) calc. 226.0724, found 226.0720



Chemical Formula: $C_{11}H_7N_5O$
Molecular Weight: 225,21