

## Supplementary Information

### **Domino Reaction of 3-Chlorochromones with Aminoheterocycles. Synthesis of Pyrazolopyridines and Benzofuropyridines and their Optical and Phosphatase Inhibitory Effects**

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#### **Content**

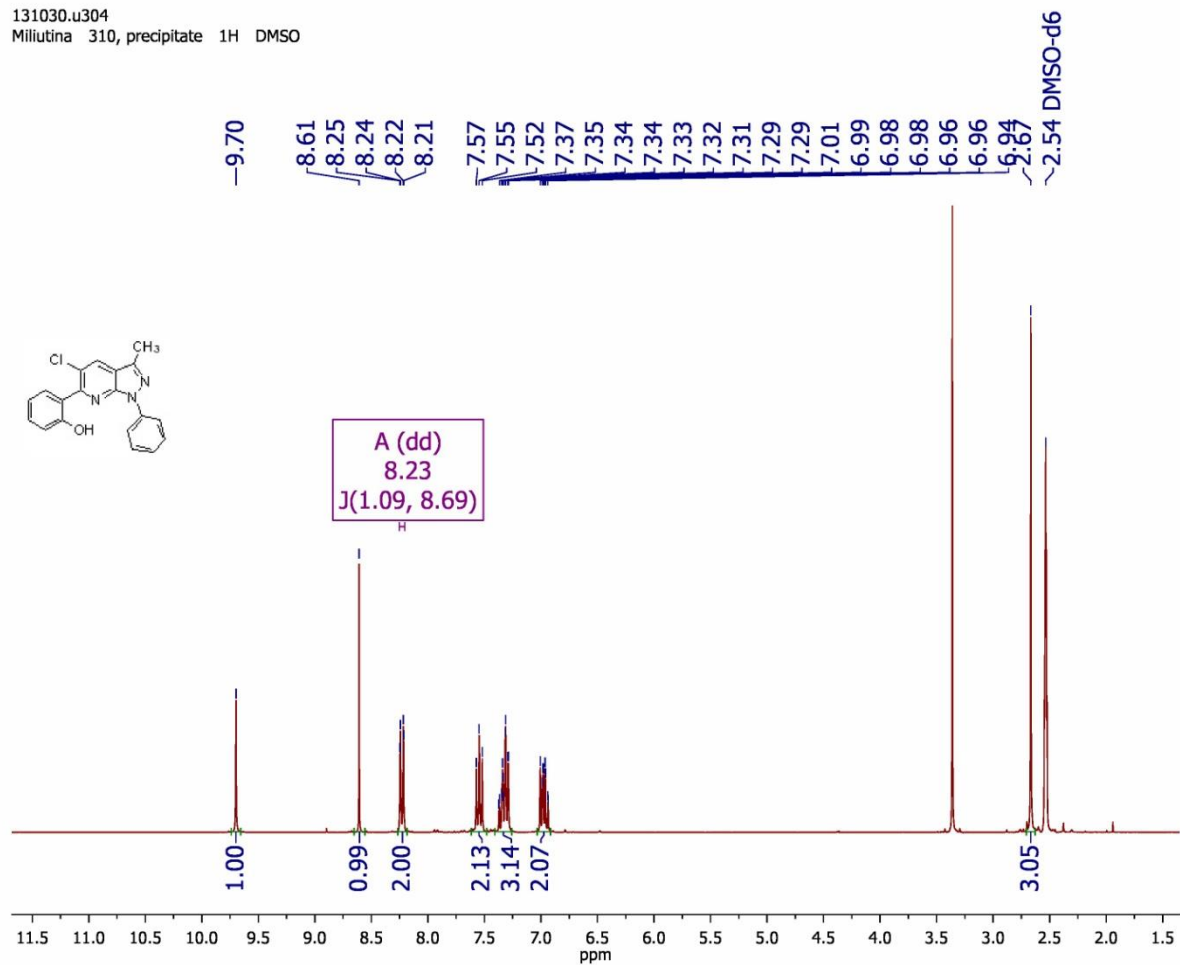
|                                                                                      |    |
|--------------------------------------------------------------------------------------|----|
| <sup>1</sup> H and <sup>13</sup> C NMR spectra of products <b>3</b> . ....           | 2  |
| <sup>1</sup> H and <sup>13</sup> C NMR spectra of products <b>4</b> . ....           | 40 |
| X-Ray structures of compounds <b>3a</b> , <b>3m</b> , <b>3o</b> and <b>4c</b> . .... | 54 |

### **<sup>1</sup>H and <sup>13</sup>C NMR spectra of products 3.**

#### **2-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (3a).**

131030.u304

Miliutina 310, precipitate 1H DMSO



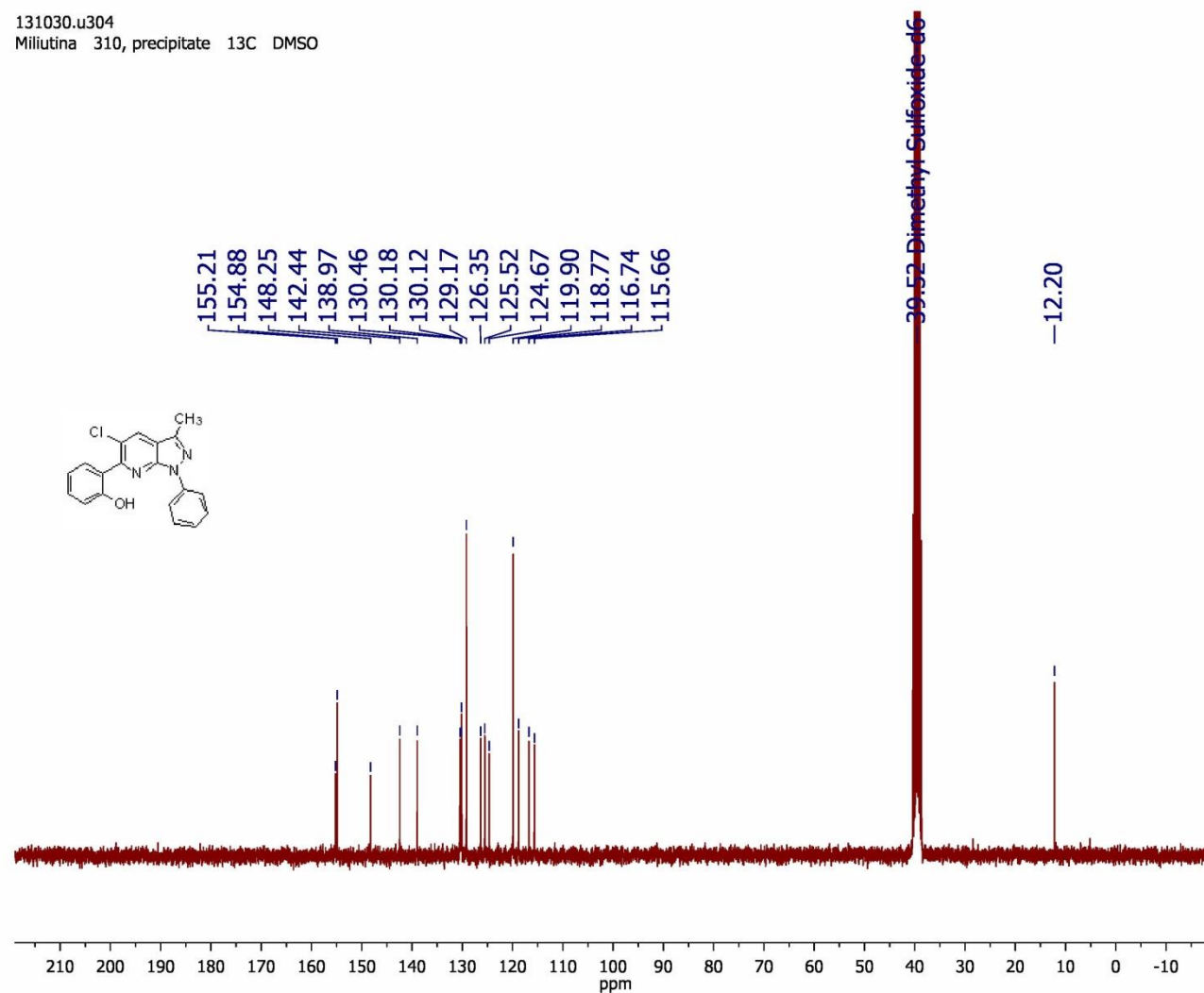
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Cl-chromone/  
m-310/  
310\_precipitate  
/ 131030.u304/  
10/ fid

Title 131030.u304  
Comment Miliutina 310,  
precipitate 1H  
DMSO  
Origin Bruker BioSpin  
GmbH  
Owner nmrsu  
Site

Spectrometer spect  
Author  
Solvent DMSO  
Temperature 298.2  
Pulse Sequence zg30  
Number of 16  
Scans  
Receiver Gain 228  
Relaxation 1.0000  
Delay  
Pulse Width 10.0000  
Acquisition Time 5.2954  
Acquisition Date 2013-10-30T08  
:20:00  
Modification 2013-10-30T08  
Date :20:04  
Spectrometer  
Frequency  
Spectral Width 6188.1  
Lowest  
Frequency  
Nucleus 1H  
Acquired Size 32768  
Spectral Size 65536

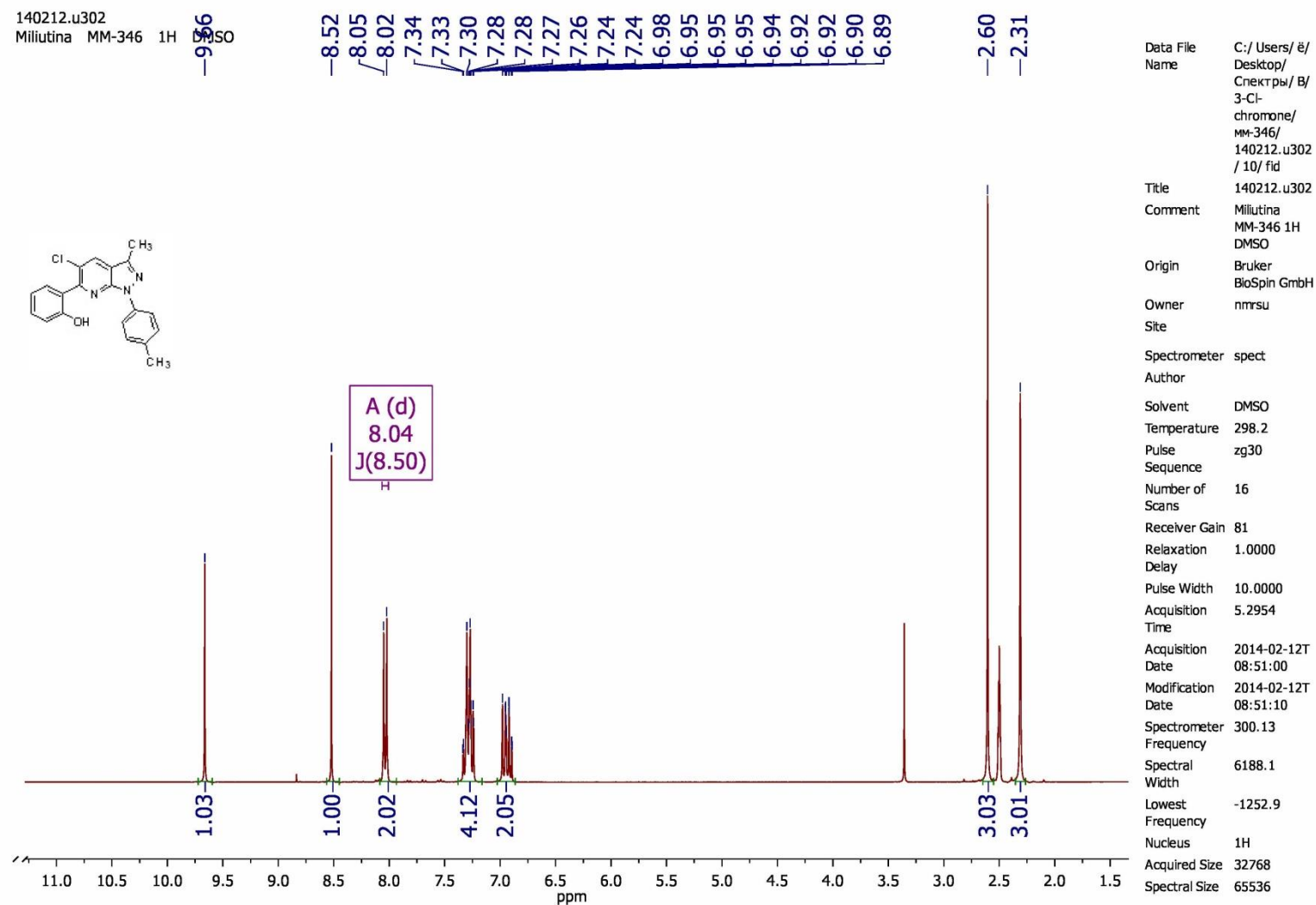
## 2-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (3a).

131030.u304  
Miliutina 310, precipitate 13C DMSO



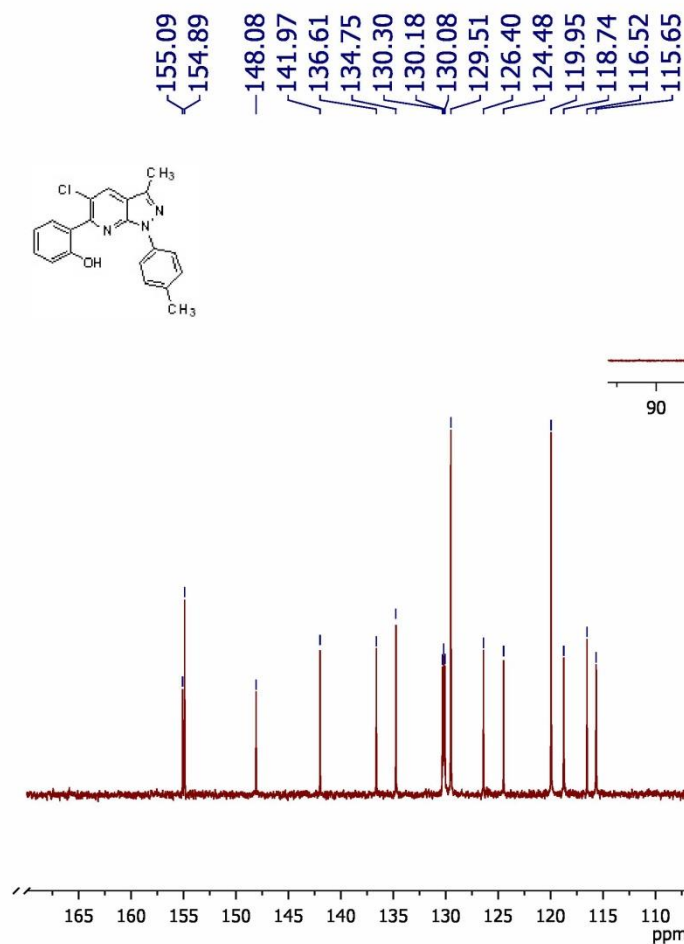
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| Title                  | 131030.u304                                                                                  |
| Comment                | Miliutina 310, precipitate 13C DMSO                                                          |
| Origin                 | Bruker BioSpin GmbH                                                                          |
| Owner                  | nmrsu                                                                                        |
| Site                   |                                                                                              |
| Spectrometer           | spect                                                                                        |
| Author                 |                                                                                              |
| Solvent                | DMSO                                                                                         |
| Temperature            | 298.2                                                                                        |
| Pulse Sequence         | zgpg30                                                                                       |
| Number of Scans        | 1024                                                                                         |
| Receiver Gain          | 2050                                                                                         |
| Relaxation Delay       | 2.0000                                                                                       |
| Pulse Width            | 10.0000                                                                                      |
| Acquisition Time       | 1.8176                                                                                       |
| Acquisition Date       | 2013-10-30T20:13:00                                                                          |
| Modification Date      | 2013-10-30T20:13:36                                                                          |
| Spectrometer Frequency | 75.47                                                                                        |
| Spectral Width         | 18028.8                                                                                      |
| Lowest Frequency       | -1506.3                                                                                      |
| Nucleus                | 13C                                                                                          |
| Acquired Size          | 32768                                                                                        |
| Spectral Size          | 65536                                                                                        |

## 2-(5-Chloro-3-methyl-1-p-tolyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (3b).



# 2-(5-Chloro-3-methyl-1-*p*-tolyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (3b).

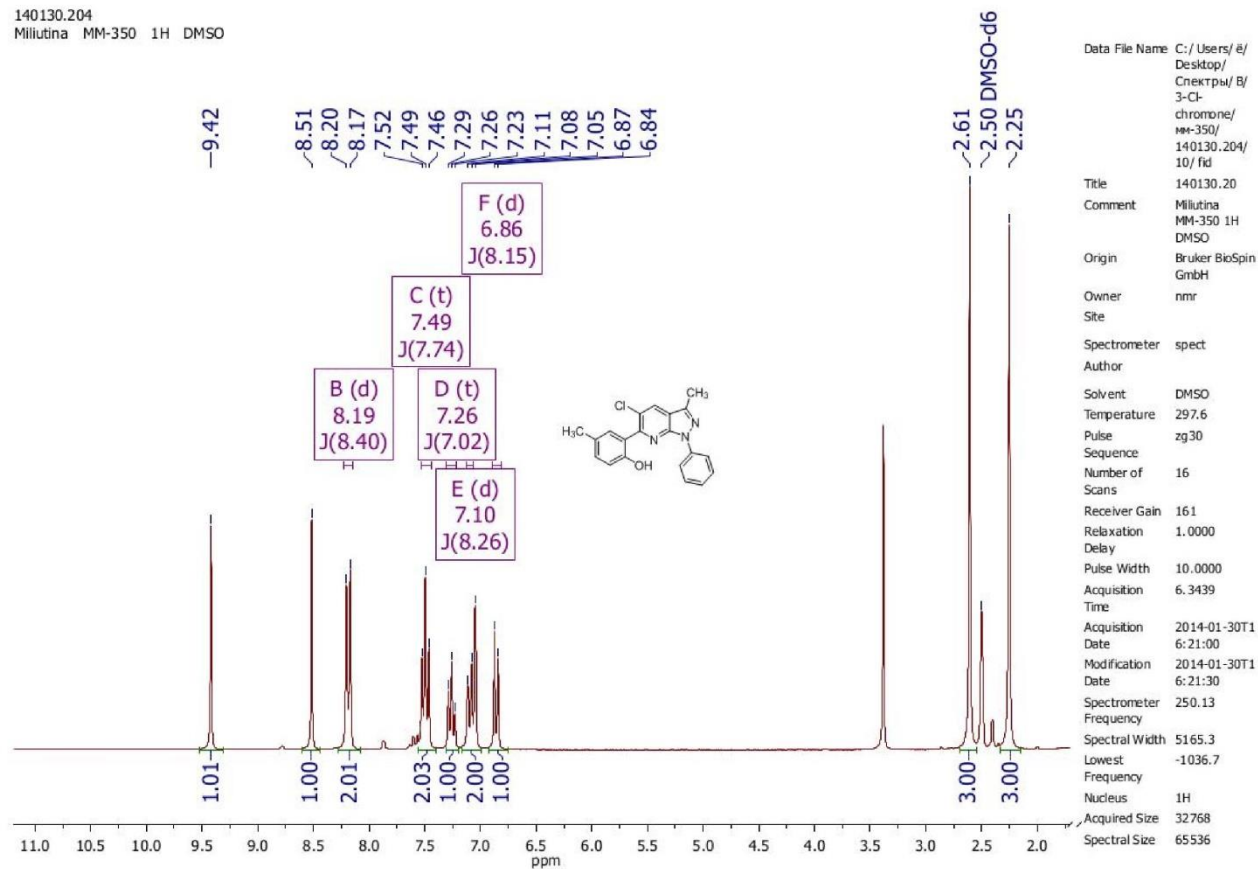
140212.205  
Millutina MM-346 13C DMSO



|                        |                                                                            |
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| Title                  | 140212.20                                                                  |
| Comment                | Millutina MM-346 13C DMSO                                                  |
| Origin                 | Bruker BioSpin GmbH                                                        |
| Owner                  | nmr                                                                        |
| Site                   |                                                                            |
| Spectrometer           | spect                                                                      |
| Author                 |                                                                            |
| Solvent                | DMSO                                                                       |
| Temperature            | 298.0                                                                      |
| Pulse Sequence         | zgpg30                                                                     |
| Number of Scans        | 1024                                                                       |
| Receiver Gain          | 2050                                                                       |
| Relaxation Delay       | 2.0000                                                                     |
| Pulse Width            | 10.0000                                                                    |
| Acquisition Time       | 2.1846                                                                     |
| Acquisition Date       | 2014-02-12T1 8:21:00                                                       |
| Modification Date      | 2014-02-12T1 8:22:14                                                       |
| Spectrometer Frequency | 62.90                                                                      |
| Spectral Width         | 15000.0                                                                    |
| Lowest Frequency       | -1240.1                                                                    |
| Nucleus                | 13C                                                                        |
| Acquired Size          | 32768                                                                      |
| Spectral Size          | 65536                                                                      |

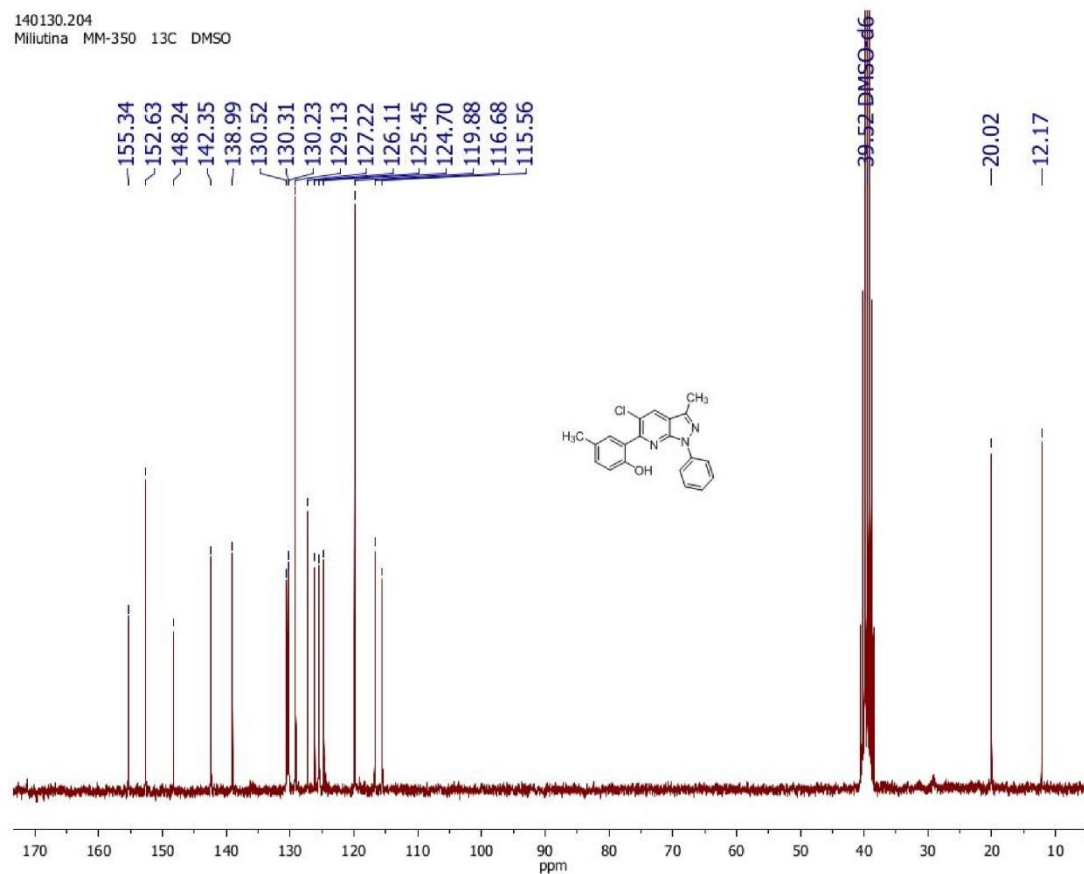
# 2-(5-Chloro-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-4-methylphenol (3c).

140130.204  
Miliutina MM-350 1H DMSO



## 2-(5-Chloro-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-4-methylphenol (3c).

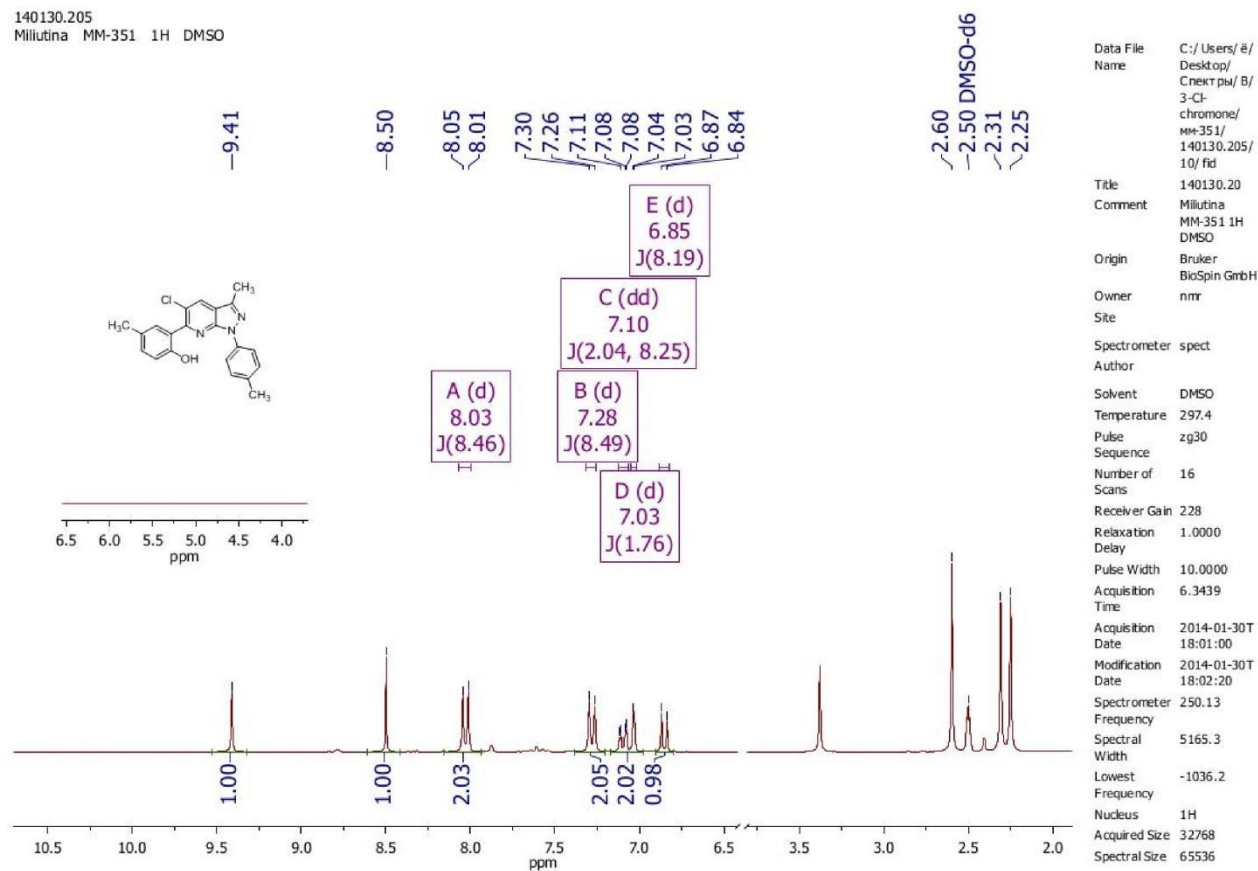
140130.204  
Miliutina MM-350 13C DMSO



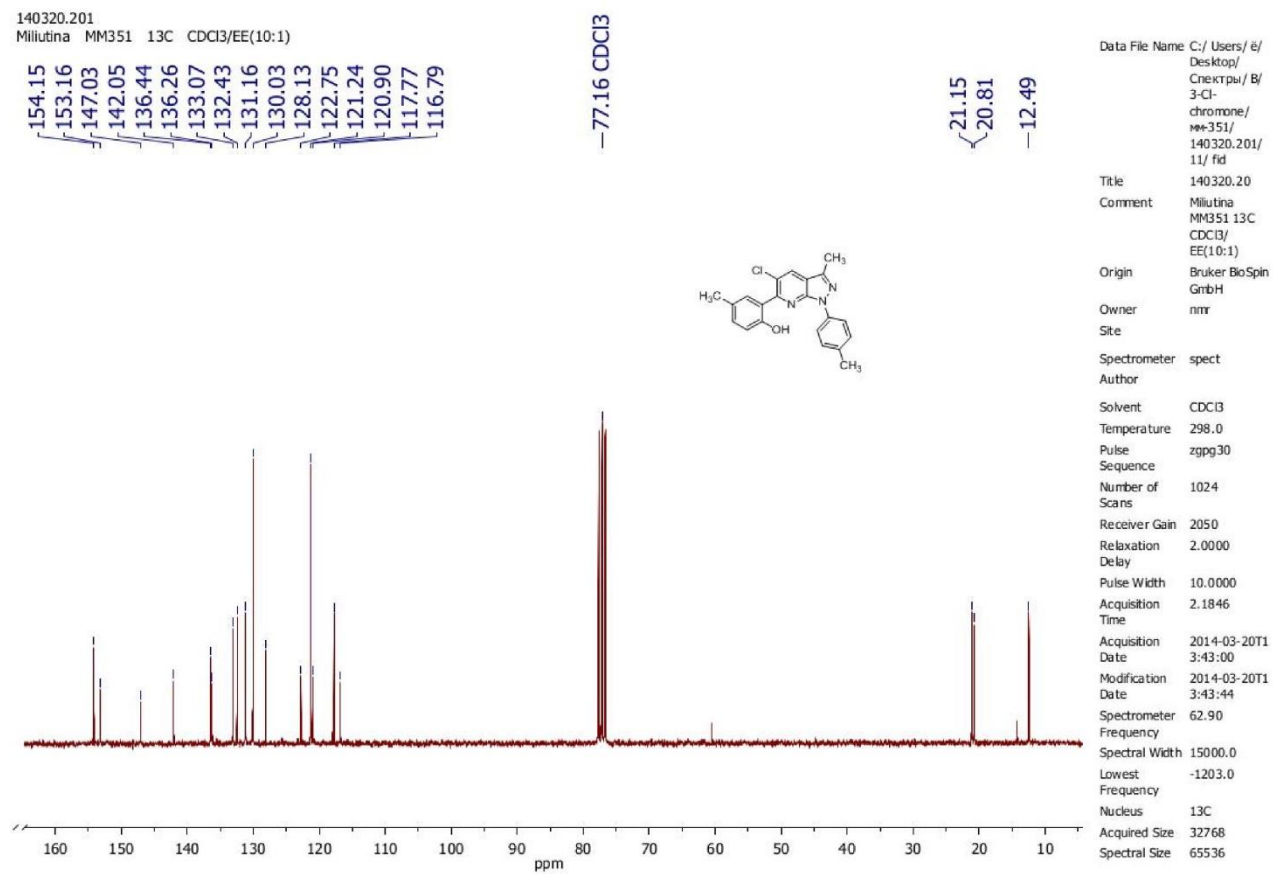
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| Title                  | 140130.20                                                                   |
| Comment                | Miliutina MM-350 13C DMSO                                                   |
| Origin                 | Bruker BioSpin GmbH                                                         |
| Owner                  | nmr                                                                         |
| Site                   |                                                                             |
| Spectrometer           | spect                                                                       |
| Author                 |                                                                             |
| Solvent                | DMSO                                                                        |
| Temperature            | 298.4                                                                       |
| Pulse                  | zgpg30                                                                      |
| Sequence               |                                                                             |
| Number of Scans        | 1024                                                                        |
| Receiver Gain          | 2050                                                                        |
| Relaxation Delay       | 2.0000                                                                      |
| Pulse Width            | 10.0000                                                                     |
| Acquisition Time       | 2.1846                                                                      |
| Acquisition Date       | 2014-01-30T 17:35:00                                                        |
| Modification Date      | 2014-01-30T 17:35:30                                                        |
| Spectrometer Frequency | 62.90                                                                       |
| Spectral Width         | 15000.0                                                                     |
| Lowest Frequency       | -1239.8                                                                     |
| Nucleus                | 13C                                                                         |
| Acquired Size          | 32768                                                                       |
| Spectral Size          | 65536                                                                       |

# 2-(5-Chloro-3-methyl-1-*p*-tolyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)-4-methylphenol (3d).

140130.205  
Miliutina MM-351 1H DMSO

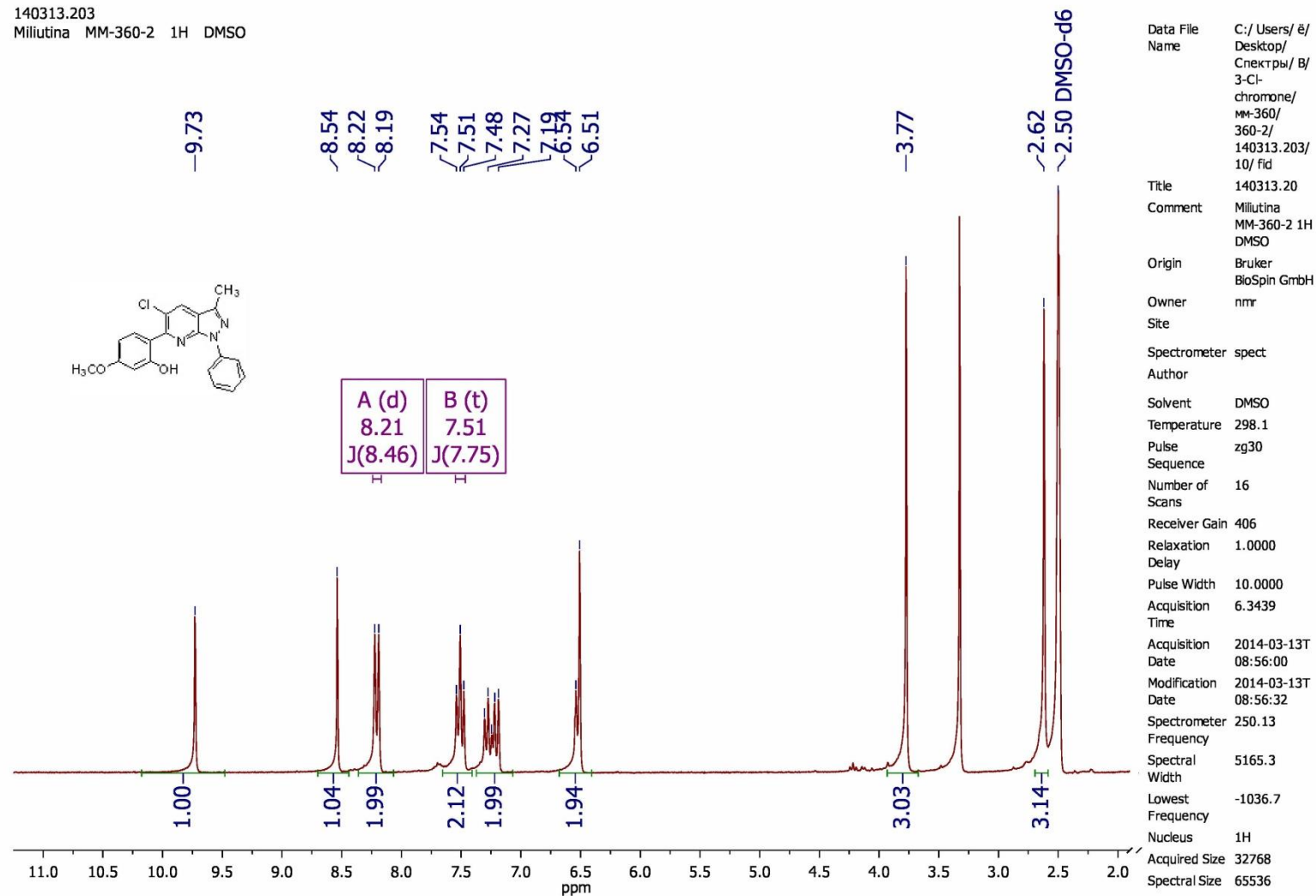


**2-(5-Chloro-3-methyl-1-*p*-tolyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)-4-methylphenol (3d).**



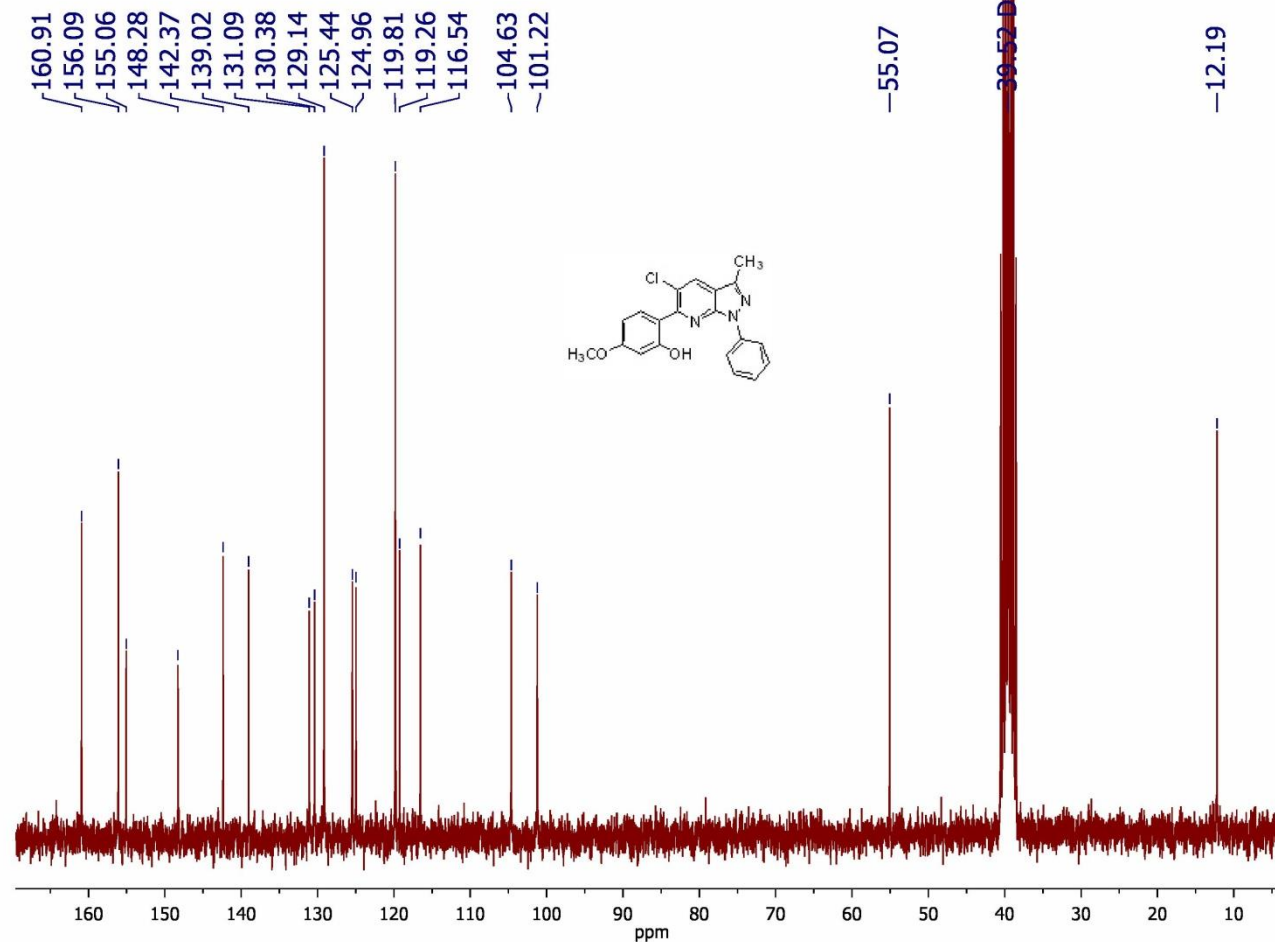
# 2-(5-Chloro-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-5-methoxyphenol (3e).

140313.203  
Millutina MM-360-2 1H DMSO



# 2-(5-Chloro-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-5-methoxyphenol (3e).

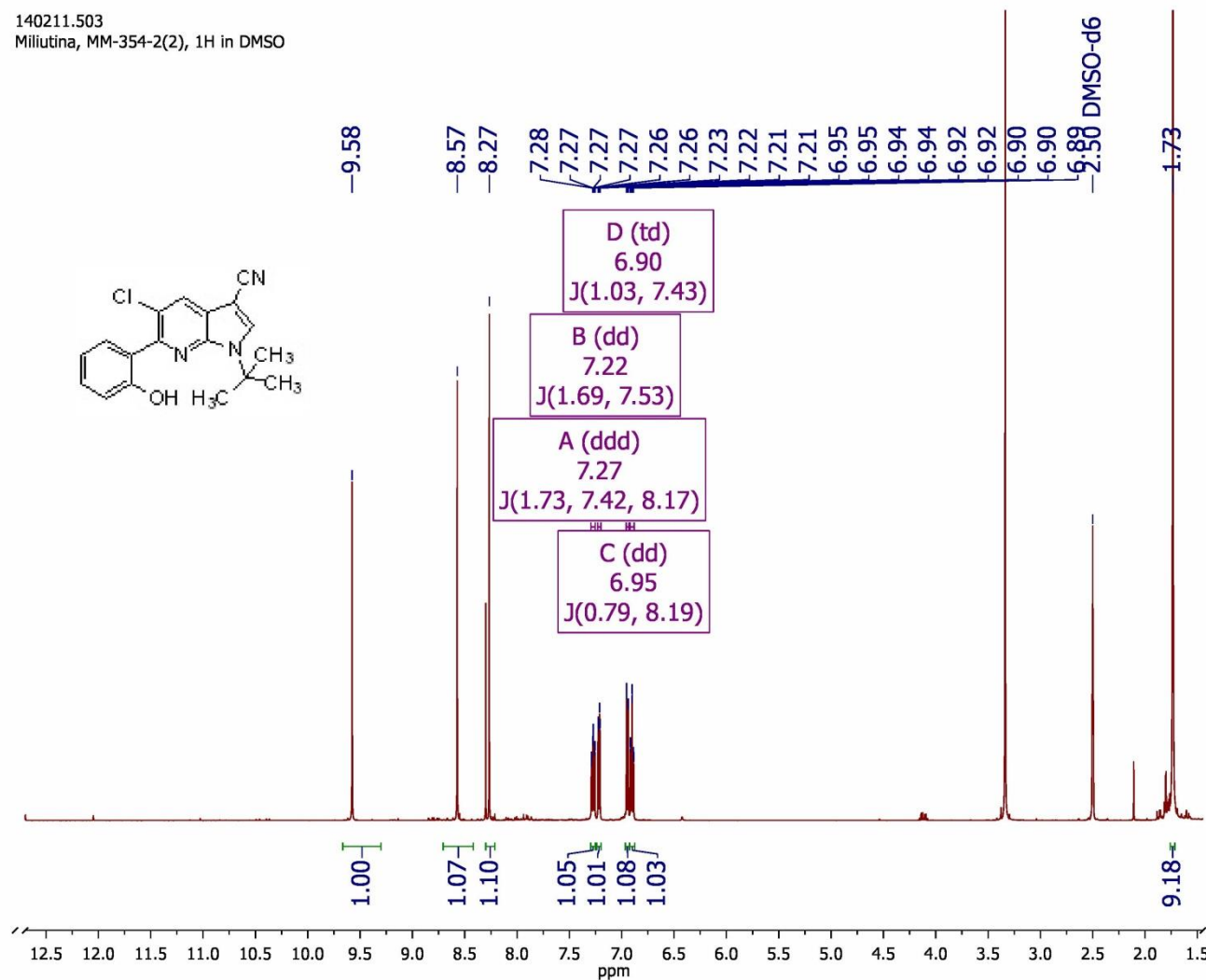
140325.204  
Miliutina MM-360.2-1 13C DMSO



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| Title                  | 140325.20                                                                          |
| Comment                | Miliutina MM-360.2-1 13C DMSO                                                      |
| Origin                 | Bruker BioSpin GmbH                                                                |
| Owner                  | nmr                                                                                |
| Site                   |                                                                                    |
| Spectrometer           | spect                                                                              |
| Author                 |                                                                                    |
| Solvent                | DMSO                                                                               |
| Temperature            | 298.0                                                                              |
| Pulse Sequence         | zgpg30                                                                             |
| Number of Scans        | 1024                                                                               |
| Receiver Gain          | 2050                                                                               |
| Relaxation Delay       | 2.0000                                                                             |
| Pulse Width            | 10.0000                                                                            |
| Acquisition Time       | 2.1846                                                                             |
| Acquisition Date       | 2014-03-26T04:07:00                                                                |
| Modification Date      | 2014-03-26T04:08:28                                                                |
| Spectrometer Frequency | 62.90                                                                              |
| Spectral Width         | 15000.0                                                                            |
| Lowest Frequency       | -1240.1                                                                            |
| Nucleus                | 13C                                                                                |
| Acquired Size          | 32768                                                                              |
| Spectral Size          | 65536                                                                              |

**1-*tert*-Butyl-5-chloro-6-(2-hydroxyphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (3g).**

140211.503  
Miliutina, MM-354-2(2), 1H in DMSO



Data File Name: C:/Users/è/Desktop/Спектры/ В/ 3-Cl- chromone/ MM-354/ 354-2(2)/ 140211.503/ 10/ fid

Title: 140211.50

Comment: Miliutina, MM-354-2(2), 1H in DMSO

Origin: Bruker BioSpin GmbH

Owner: Administrator

Site:

Spectrometer: spect

Author:

Solvent: DMSO

Temperature: 300.1

Pulse Sequence: zg30

Number of Scans: 32

Receiver Gain: 114

Relaxation Delay: 1.0000

Pulse Width: 9.8000

Acquisition Time: 3.1720

Acquisition Date: 2014-02-11T1 5:03:00

Modification Date: 2014-02-11T1 5:04:08

Spectrometer Frequency: 500.13

Spectral Width: 10330.6

Lowest Frequency: -2081.8

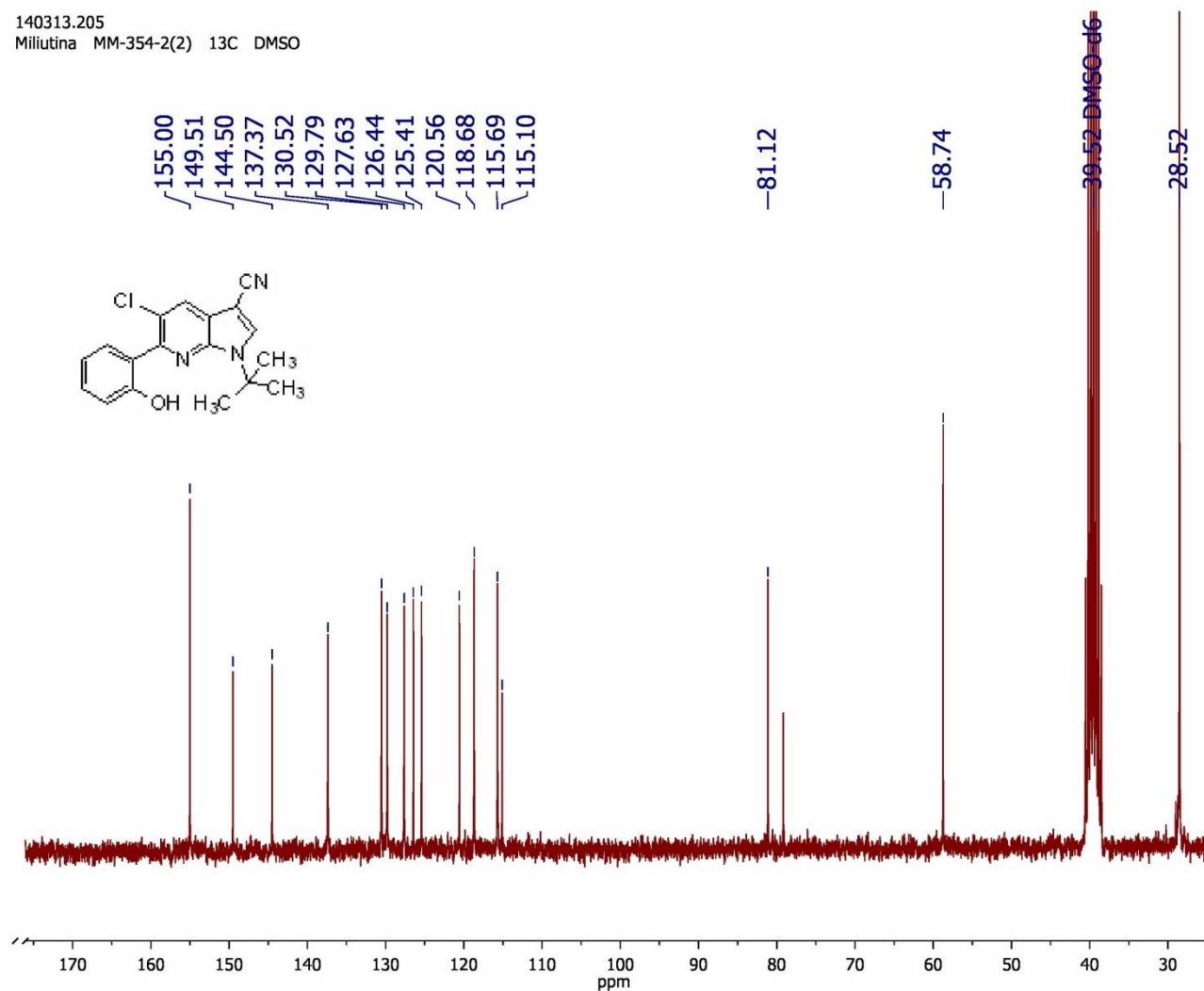
Nucleus: 1H

Acquired Size: 32768

Spectral Size: 65536

**1-*tert*-Butyl-5-chloro-6-(2-hydroxyphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (3g).**

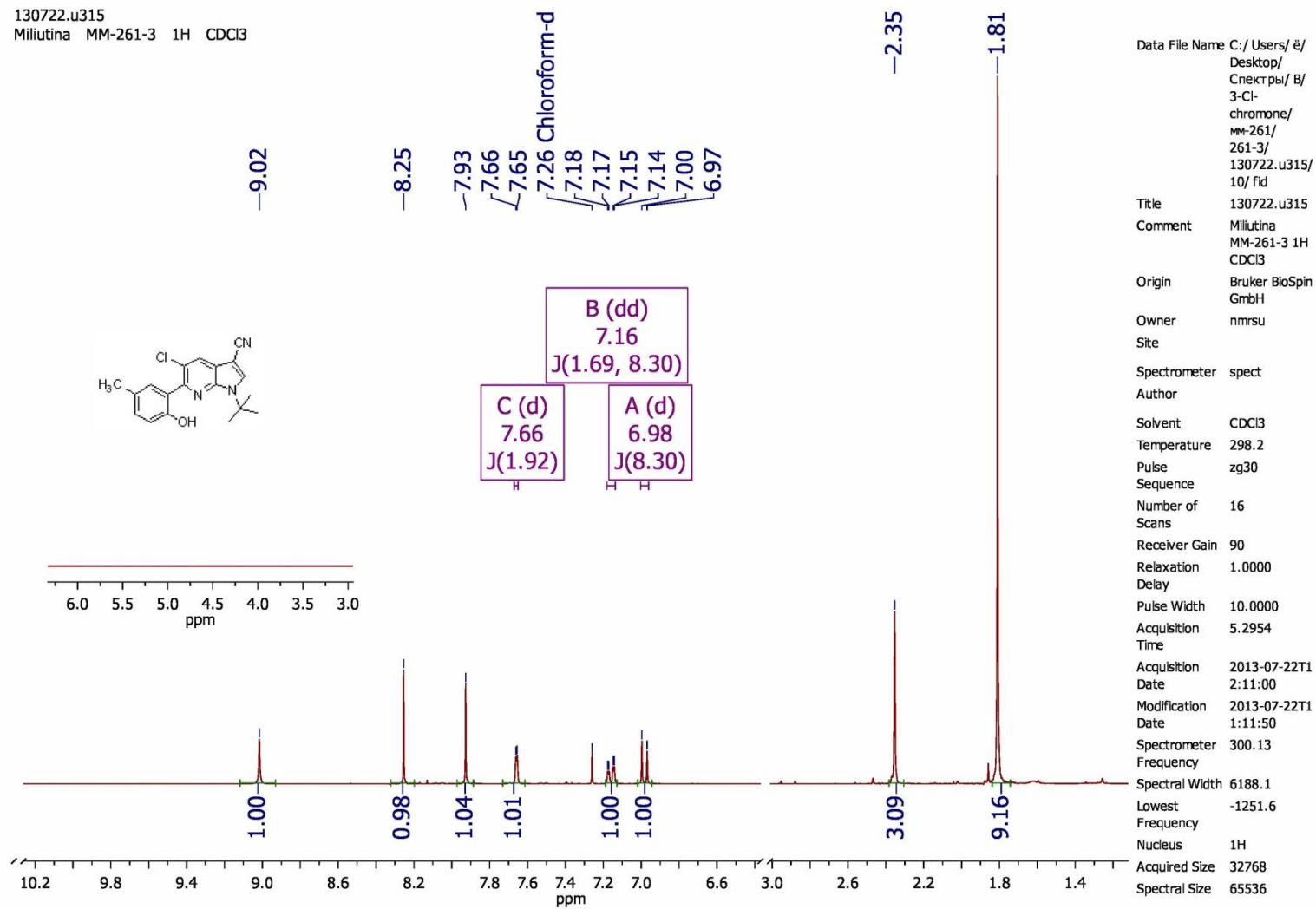
140313.205  
Millutina MM-354-2(2) 13C DMSO



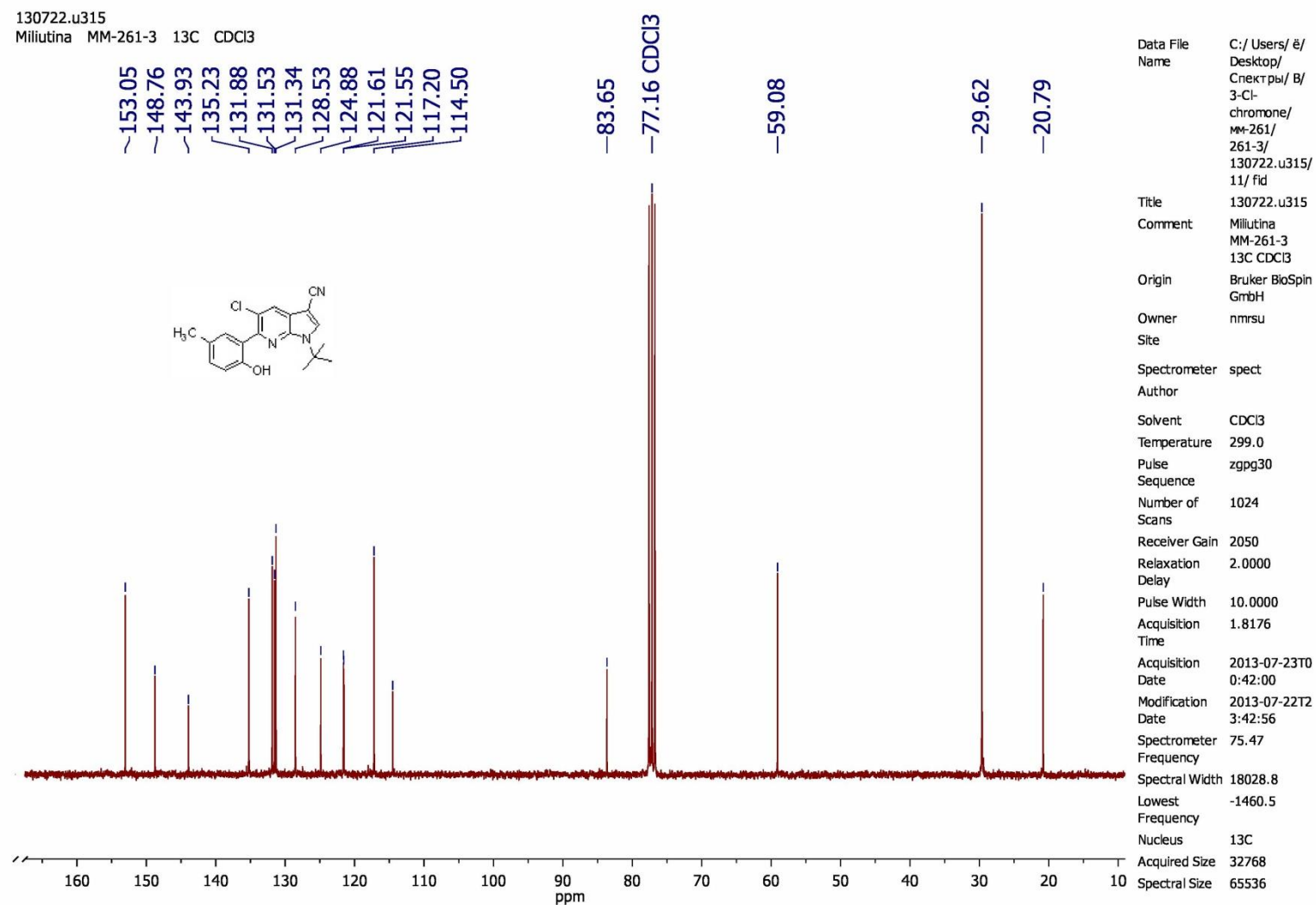
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| Title                  | 140313.20                                                                            |
| Comment                | Millutina MM-354-2(2) 13C DMSO                                                       |
| Origin                 | Bruker BioSpin GmbH                                                                  |
| Owner                  | nmr                                                                                  |
| Site                   |                                                                                      |
| Spectrometer           | spect                                                                                |
| Author                 |                                                                                      |
| Solvent                | DMSO                                                                                 |
| Temperature            | 298.0                                                                                |
| Pulse Sequence         | zgpg30                                                                               |
| Number of Scans        | 1024                                                                                 |
| Receiver Gain          | 2050                                                                                 |
| Relaxation Delay       | 2.0000                                                                               |
| Pulse Width            | 10.0000                                                                              |
| Acquisition Time       | 2.1846                                                                               |
| Acquisition Date       | 2014-03-13T12:10:00                                                                  |
| Modification Date      | 2014-03-13T12:11:24                                                                  |
| Spectrometer Frequency | 62.90                                                                                |
| Spectral Width         | 15000.0                                                                              |
| Lowest Frequency       | -1240.1                                                                              |
| Nucleus                | 13C                                                                                  |
| Acquired Size          | 32768                                                                                |
| Spectral Size          | 65536                                                                                |

**1-*tert*-Butyl-5-chloro-6-(2-hydroxy-5-methylphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (3h).**

130722.u315  
Miliutina MM-261-3 1H CDCl<sub>3</sub>

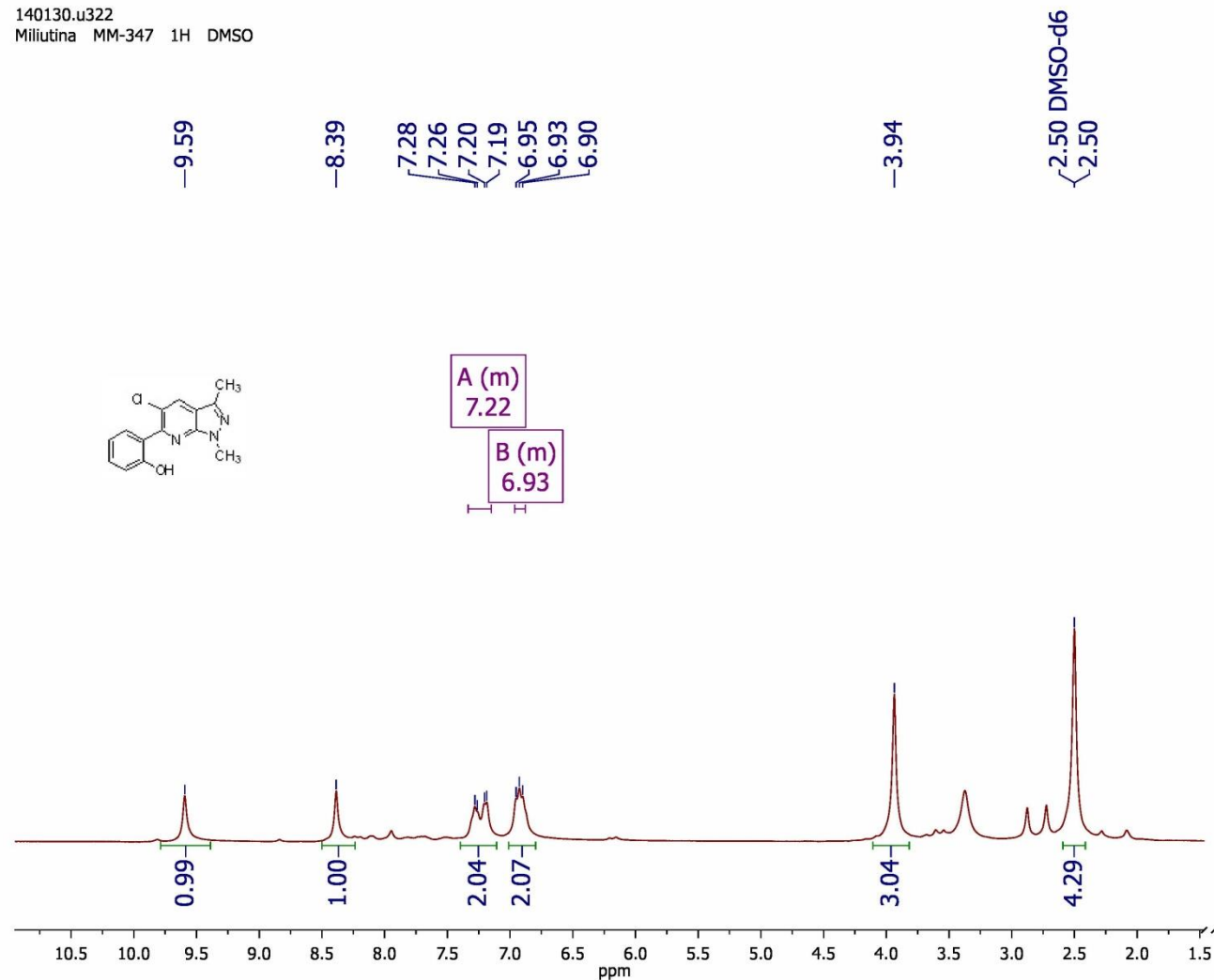


**1-*tert*-Butyl-5-chloro-6-(2-hydroxy-5-methylphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (3h).**



## 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (3i).

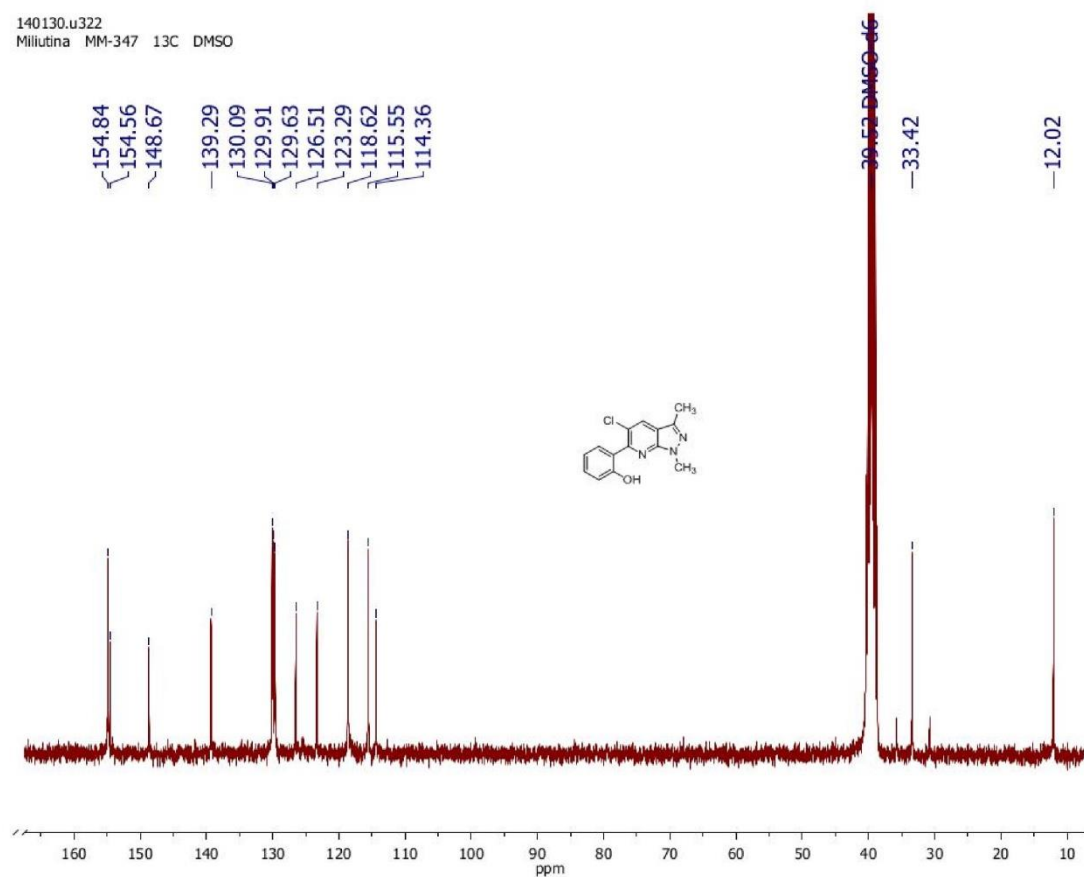
140130.u322  
Miliutina MM-347 1H DMSO



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Comment: Miliutina MM-347 1H DMSO  
Origin: Bruker BioSpin GmbH  
Owner: nmrsu  
Site:  
Spectrometer: spect  
Author:  
Solvent: DMSO  
Temperature: 298.2  
Pulse Sequence: zg30  
Number of Scans: 16  
Receiver Gain: 81  
Relaxation Delay: 1.0000  
Pulse Width: 10.0000  
Acquisition Time: 5.2954  
Acquisition Date: 2014-01-30T21:03:00  
Modification Date: 2014-01-30T21:03:48  
Spectrometer Frequency: 300.13  
Spectral Width: 6188.1  
Lowest Frequency: -1278.5  
Nucleus: 1H  
Acquired Size: 32768  
Spectral Size: 65536

## 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (3i).

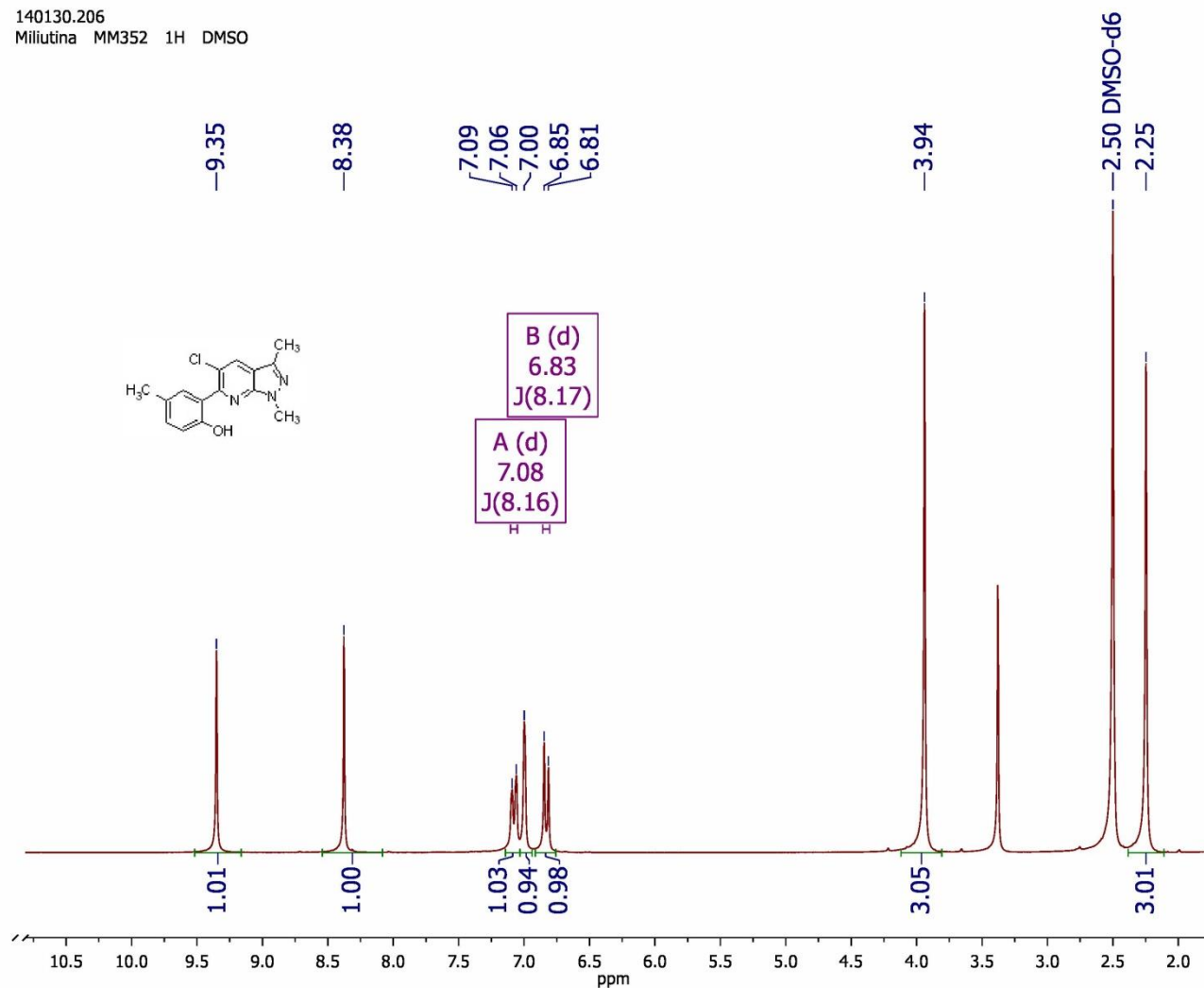
140130.u322  
Miliutina MM-347 13C DMSO



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|                   | chromone/      |
|                   | MM-347/        |
|                   | 140130.u322/   |
|                   | 11/ fid        |
| Title             | 140130.u322    |
| Comment           | Miliutina      |
|                   | MM-347 13C     |
|                   | DMSO           |
| Origin            | Bruker BioSpin |
| Owner             | GmbH           |
| Site              | nmrsu          |
| Spectrometer      | spect          |
| Author            |                |
| Solvent           | DMSO           |
| Temperature       | 298.2          |
| Pulse             | zgpg30         |
| Sequence          |                |
| Number of Scans   | 1024           |
| Receiver Gain     | 2050           |
| Relaxation Delay  | 2.0000         |
| Pulse Width       | 10.0000        |
| Acquisition Time  | 1.8176         |
| Acquisition Date  | 2014-01-30T2   |
|                   | 2:11:00        |
| Modification Date | 2014-01-30T2   |
|                   | 2:11:38        |
| Spectrometer      | 75.47          |
| Frequency         |                |
| Spectral Width    | 18028.8        |
| Lowest            | -1510.7        |
| Frequency         |                |
| Nucleus           | 13C            |
| Acquired Size     | 32768          |
| Spectral Size     | 65536          |

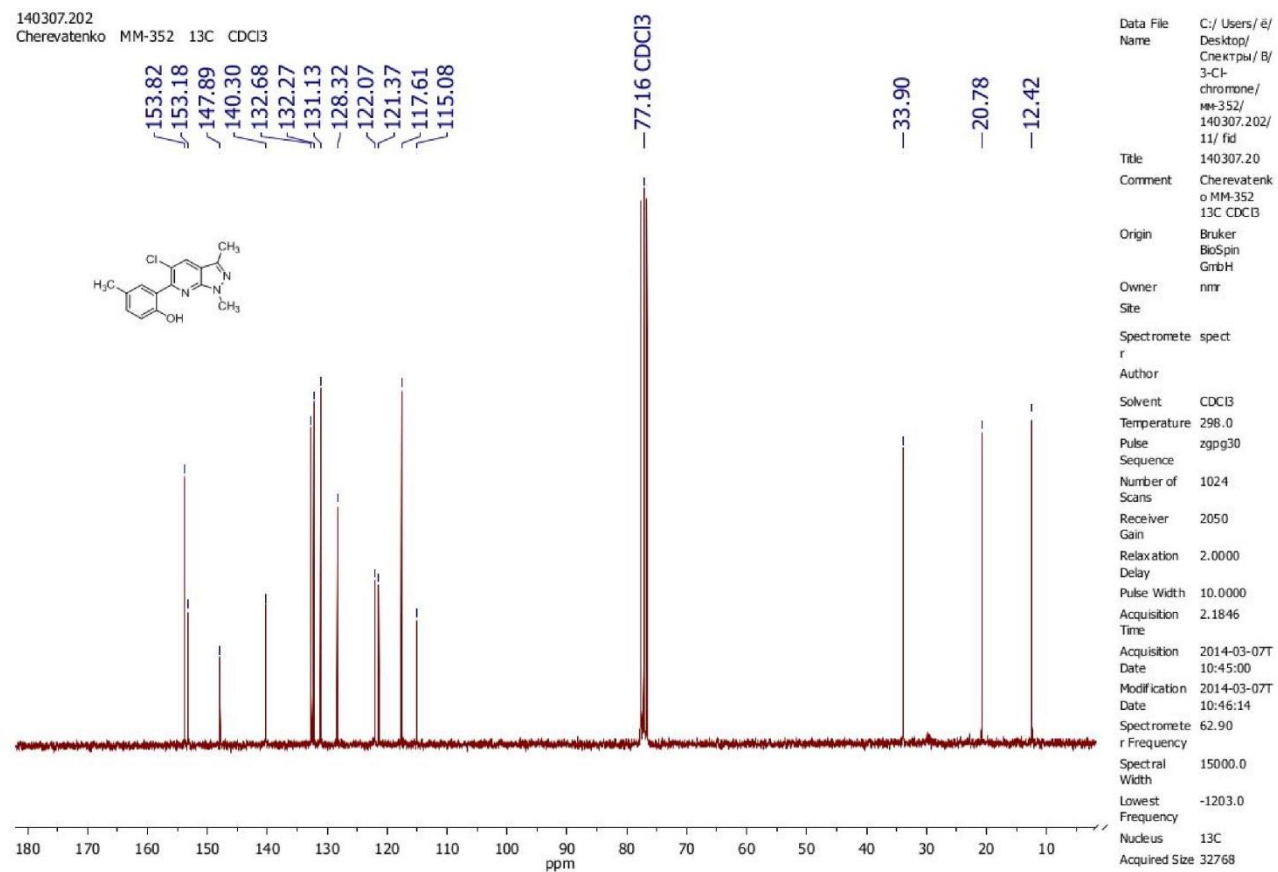
# 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-4-methylphenol (3j).

140130.206  
Miliutina MM352 1H DMSO



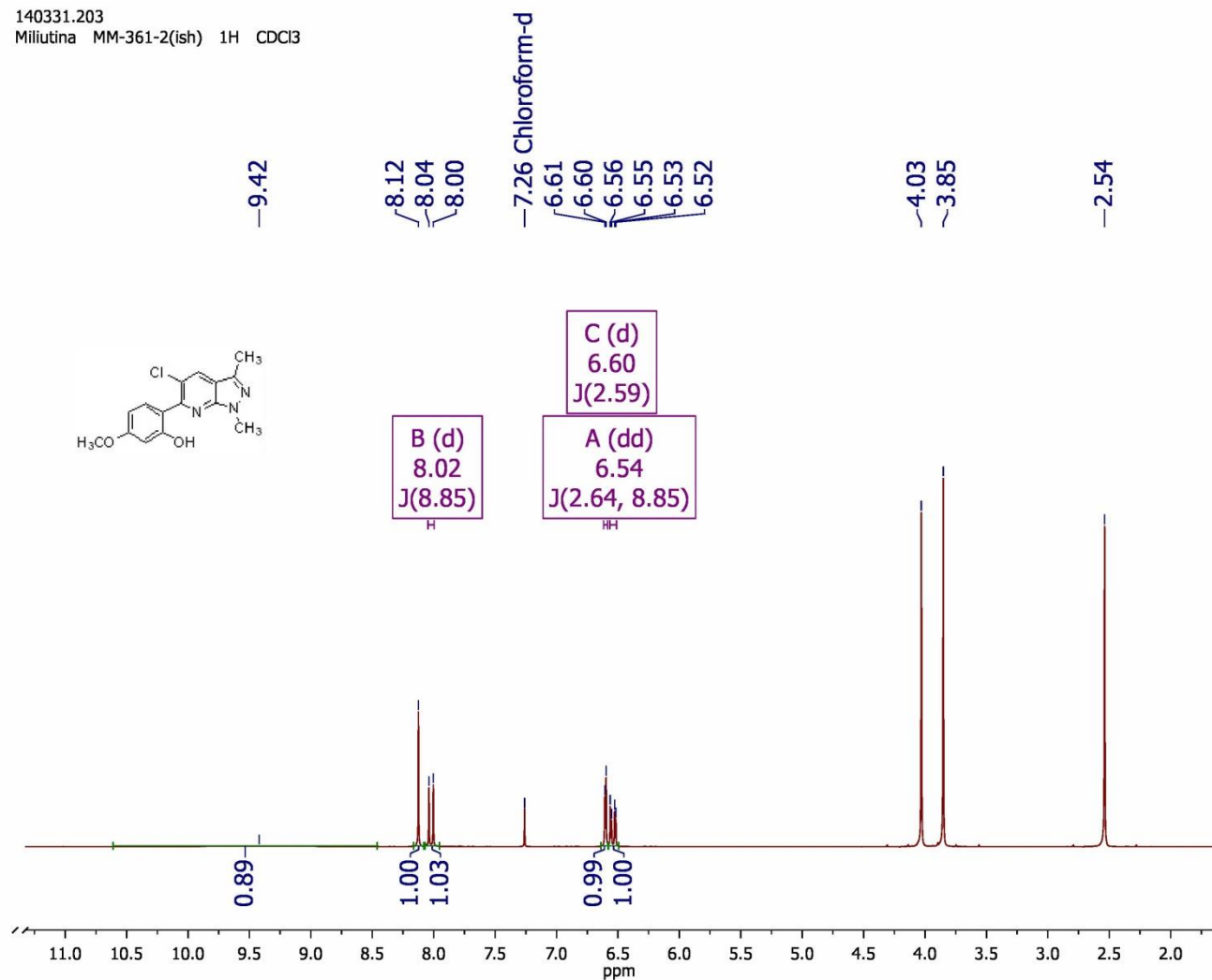
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| Title                  | 140130.21                                                                 |
| Comment                | Miliutina MM352 1H DMSO                                                   |
| Origin                 | Bruker BioSpin GmbH                                                       |
| Owner                  | nmr                                                                       |
| Site                   |                                                                           |
| Spectrometer           | spect                                                                     |
| Author                 |                                                                           |
| Solvent                | DMSO                                                                      |
| Temperature            | 297.0                                                                     |
| Pulse                  | zg30                                                                      |
| Sequence               |                                                                           |
| Number of Scans        | 16                                                                        |
| Receiver Gain          | 228                                                                       |
| Relaxation Delay       | 1.0000                                                                    |
| Pulse Width            | 10.0000                                                                   |
| Acquisition Time       | 6.3439                                                                    |
| Acquisition Date       | 2014-01-31T00:31:00                                                       |
| Modification Date      | 2014-01-31T00:31:46                                                       |
| Spectrometer Frequency | 250.13                                                                    |
| Spectral Width         | 5165.3                                                                    |
| Lowest Frequency       | -1035.8                                                                   |
| Nucleus                | 1H                                                                        |
| Acquired Size          | 32768                                                                     |
| Spectral Size          | 65536                                                                     |

## 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-*b*]pyridin-6-yl)-4-methylphenol (3j).



# 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-5-methoxyphenol (3k).

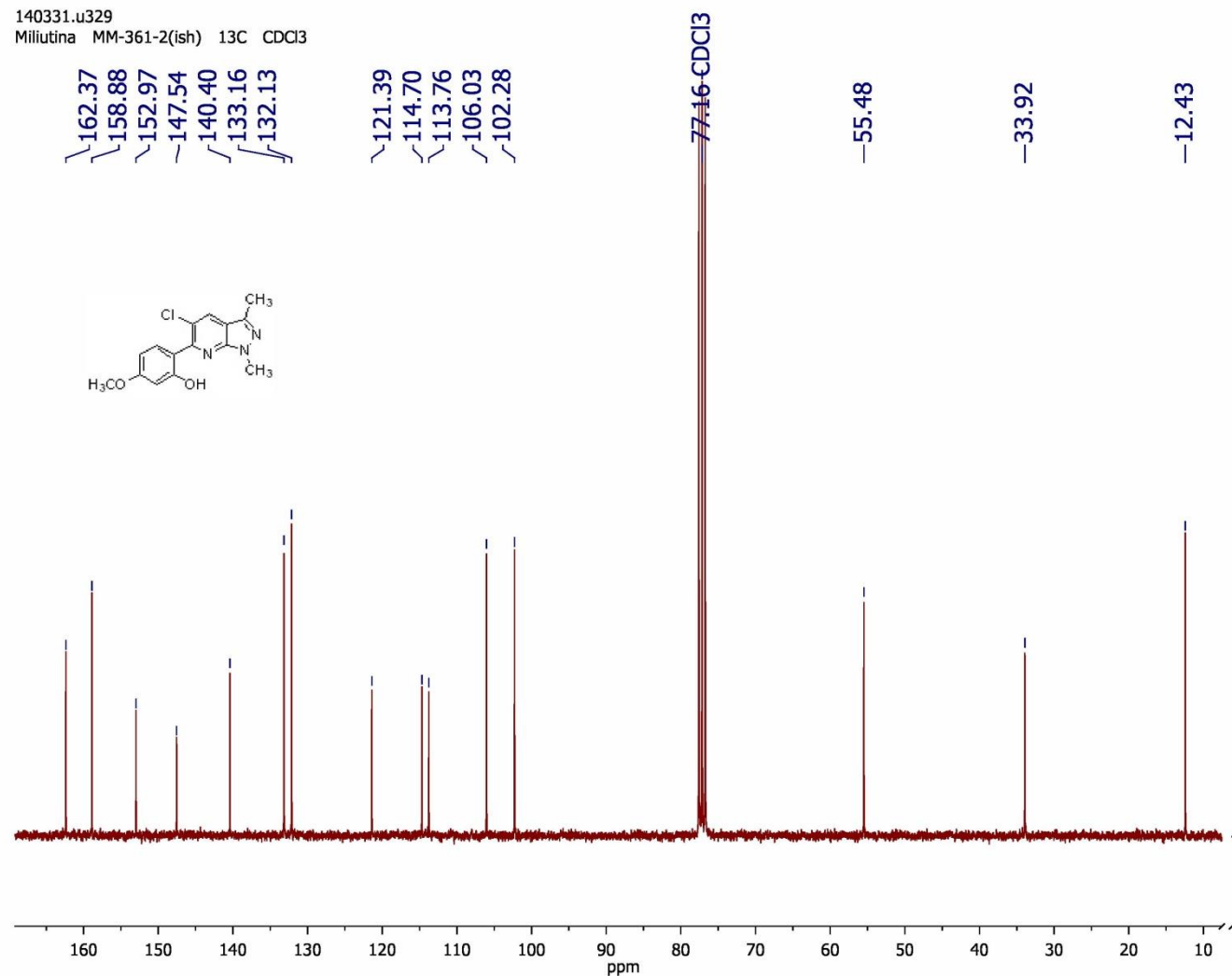
140331.203  
Miliutina MM-361-2(ish) 1H CDCl3



Data File Name C:/Users/ë/Desktop/Спектры/ B/3-Cl-chromone/MM-361/361-2/140331.203/10/ fid  
Title 140331.20  
Comment Miliutina MM-361-2(ish) 1H CDCl3  
Origin Bruker BioSpin GmbH  
Owner nmr  
Site  
Spectrometer spect  
Author  
Solvent CDCl3  
Temperature 298.1  
Pulse zg30  
Sequence  
Number of Scans 16  
Receiver Gain 362  
Relaxation 1.0000  
Delay  
Pulse Width 10.0000  
Acquisition Time 6.3439  
Acquisition Date 2014-03-31T1 3:03:00  
Modification Date 2014-03-31T1 2:03:26  
Spectrometer Frequency 250.13  
Spectral Width 5165.3  
Lowest Frequency -1038.4  
Nucleus 1H  
Acquired Size 32768  
Spectral Size 65536

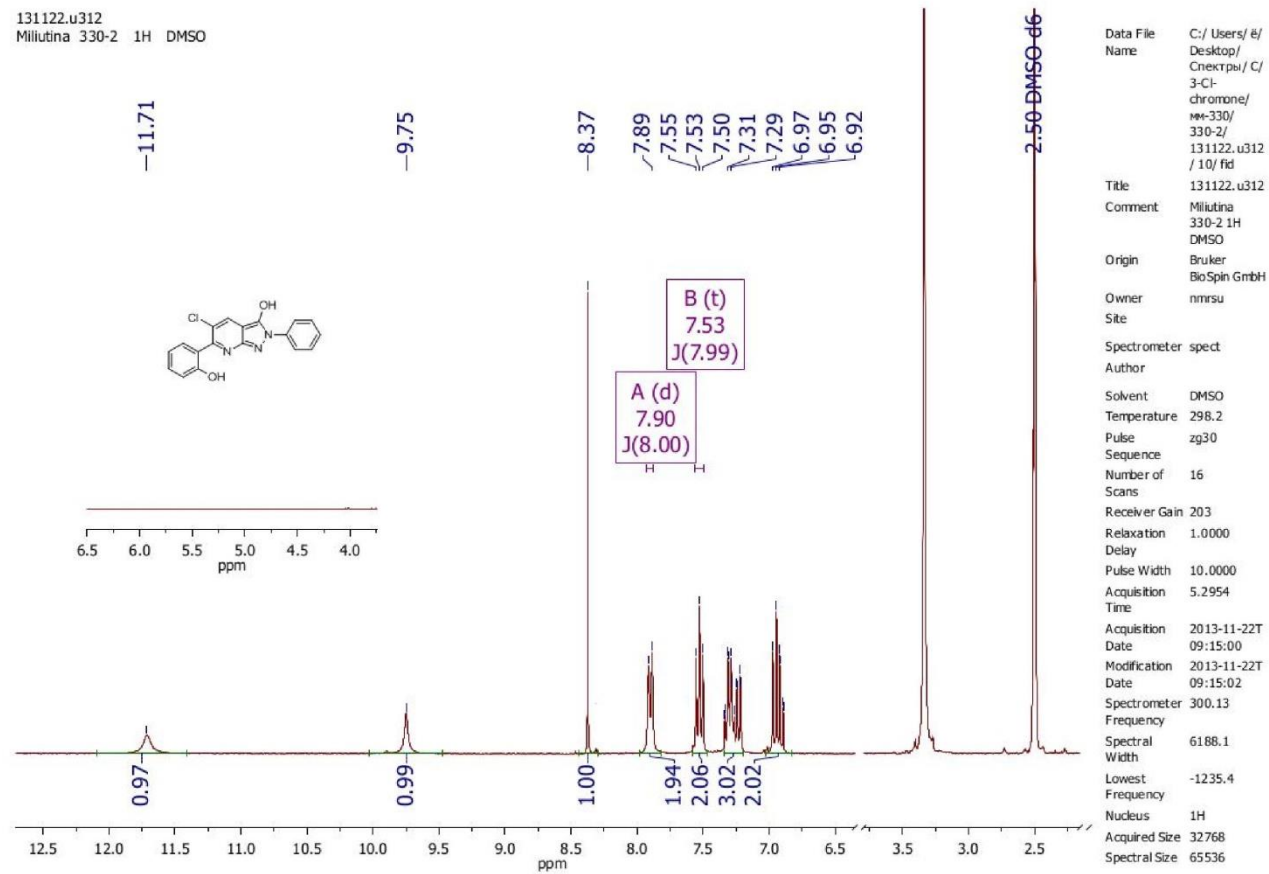
# 2-(5-Chloro-1,3-dimethyl-1H-pyrazolo[3,4-b]pyridin-6-yl)-5-methoxyphenol (3k).

140331.u329  
Miliutina MM-361-2(ish) 13C CDCl3



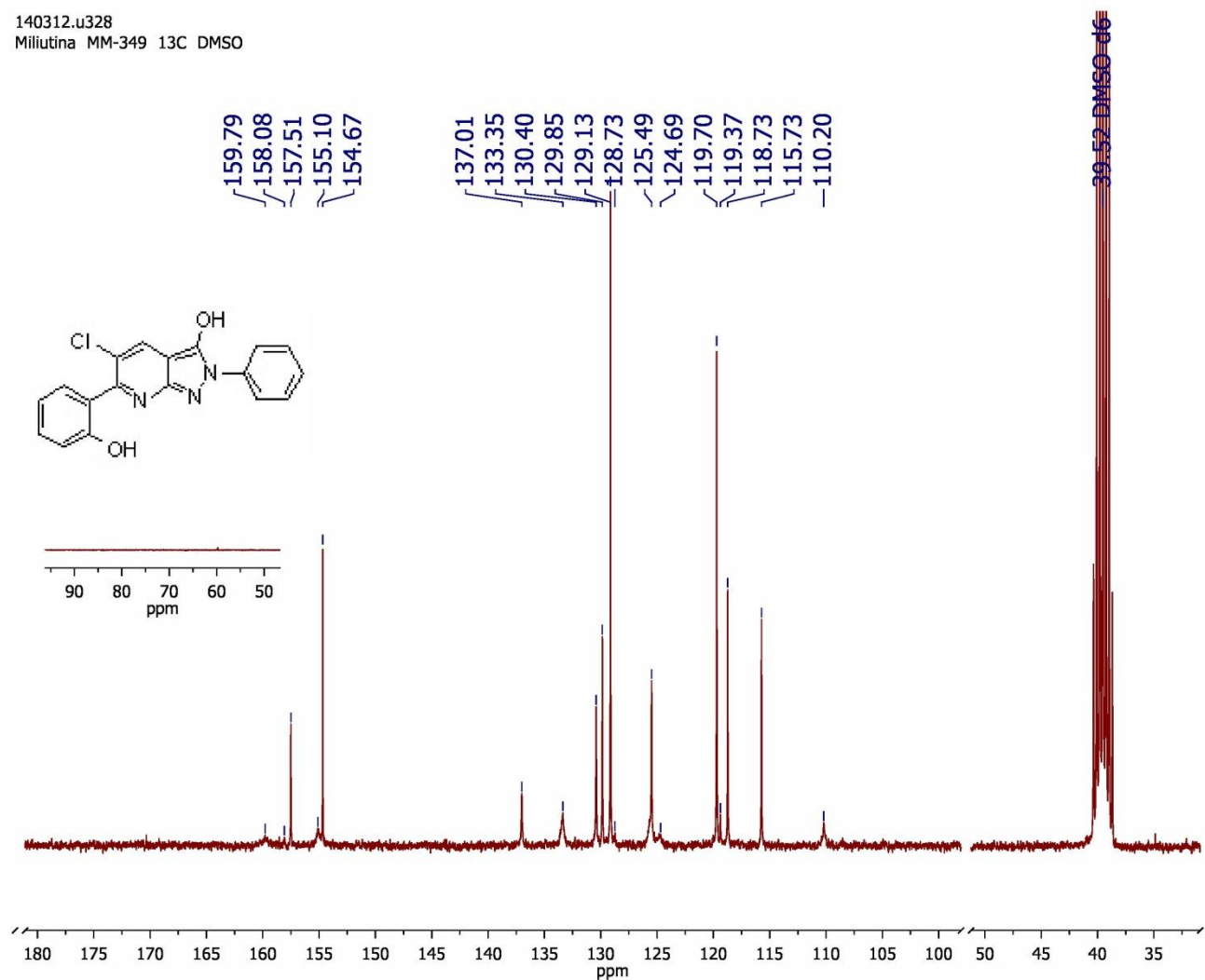
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| Title                  | 140331.u329                                                                         |
| Comment                | Miliutina MM-361-2(ish) 13C CDCl3                                                   |
| Origin                 | Bruker BioSpin GmbH                                                                 |
| Owner                  | nmsu                                                                                |
| Site                   |                                                                                     |
| Spectrometer           | spect                                                                               |
| Author                 |                                                                                     |
| Solvent                | CDCl3                                                                               |
| Temperature            | 298.2                                                                               |
| Pulse Sequence         | zgpg30                                                                              |
| Number of Scans        | 1024                                                                                |
| Receiver Gain          | 2050                                                                                |
| Relaxation Delay       | 2.0000                                                                              |
| Pulse Width            | 10.0000                                                                             |
| Acquisition Time       | 1.8176                                                                              |
| Acquisition Date       | 2014-04-01T 00:10:00                                                                |
| Modification Date      | 2014-03-31T 23:10:02                                                                |
| Spectrometer Frequency | 75.47                                                                               |
| Spectral Width         | 18028.8                                                                             |
| Lowest Frequency       | -1460.0                                                                             |
| Nucleus                | 13C                                                                                 |
| Acquired Size          | 32768                                                                               |
| Spectral Size          | 65536                                                                               |

# 5-Chloro-6-(2-hydroxyphenyl)-2-phenyl-2H-pyrazolo[3,4-*b*]pyridin-3-ol (31).



# 5-Chloro-6-(2-hydroxyphenyl)-2-phenyl-2H-pyrazolo[3,4-*b*]pyridin-3-ol (3l).

140312.u328  
Millutina MM-349 13C DMSO



Data File Name: C:/Users/è/Desktop/Спектры/ В/ 3-Cl-chromone/ мм-349/ 140312.u328/ 11/ fid

Title: 140312.u328

Comment: Millutina MM-349 13C DMSO

Origin: Bruker BioSpin GmbH

Owner: nmrsu

Site:

Spectrometer: spect

Author:

Solvent: DMSO

Temperature: 298.2

Pulse: zgpg30

Sequence:

Number of Scans: 2048

Receiver Gain: 2050

Relaxation Delay: 2.0000

Pulse Width: 10.0000

Acquisition Time: 1.8176

Acquisition Date: 2014-03-12T1 8:15:00

Modification Date: 2014-03-12T1 8:16:00

Spectrometer Frequency: 75.47

Spectral Width: 18028.8

Lowest Frequency: -1505.7

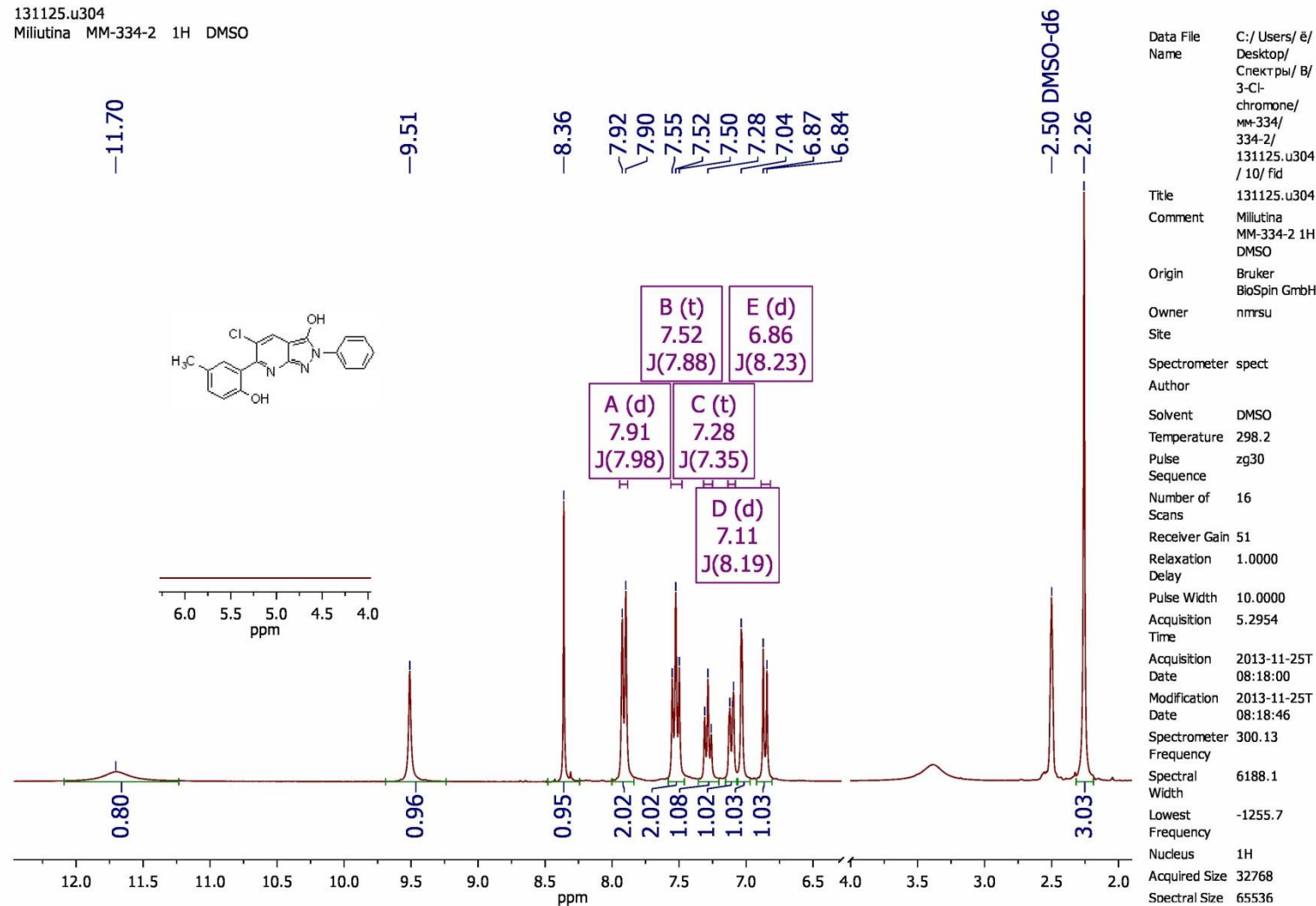
Nucleus: 13C

Acquired Size: 32768

Spectral Size: 65536

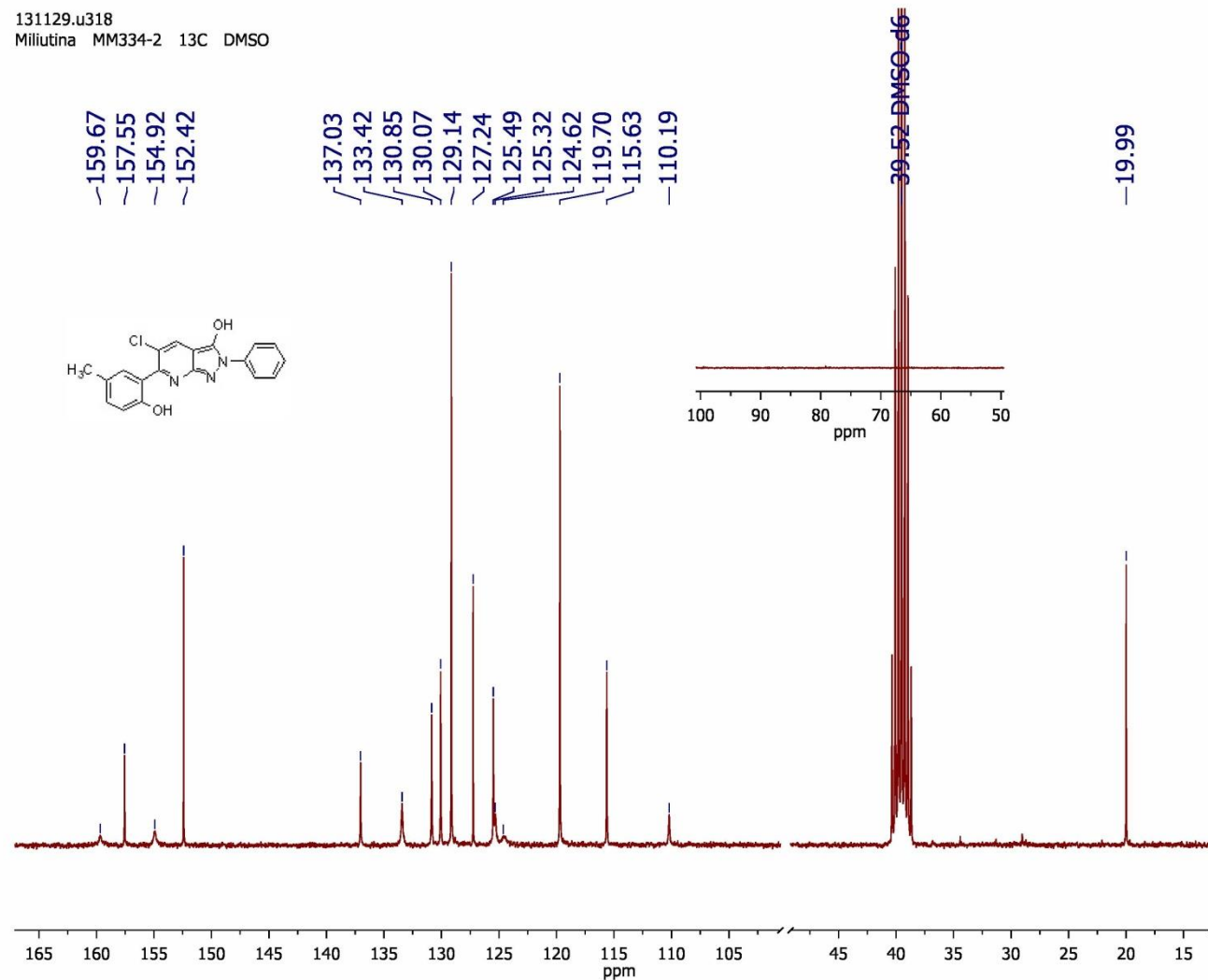
# 5-Chloro-6-(2-hydroxy-5-methylphenyl)-2-phenyl-2H-pyrazolo[3,4-*b*]pyridin-3-ol (3m).

131125.u304  
Miliutina MM-334-2 1H DMSO



# 5-Chloro-6-(2-hydroxy-5-methylphenyl)-2-phenyl-2H-pyrazolo[3,4-b]pyridin-3-ol (3m).

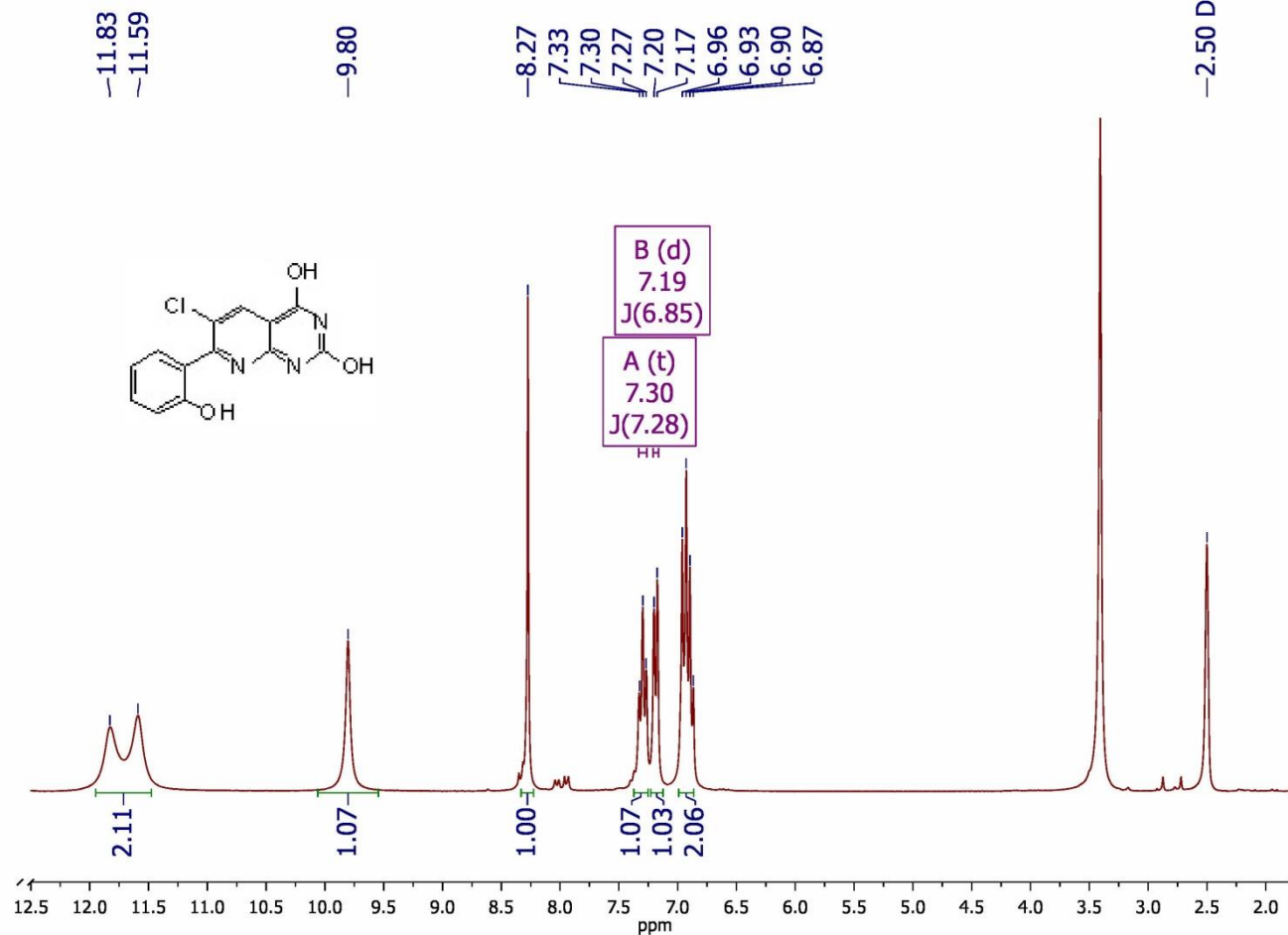
131129.u318  
Miliutina MM334-2 13C DMSO



|                        |                                                                                     |
|------------------------|-------------------------------------------------------------------------------------|
| Data File Name         | C:/Users/ё/Desktop/Спектры/ B/ 3-Cl- chromone/ мм-334/ 334-2/ 131129.u318 / 10/ fid |
| Title                  | 131129.u318                                                                         |
| Comment                | Miliutina MM334-2 13C DMSO                                                          |
| Origin                 | Bruker BioSpin GmbH                                                                 |
| Owner                  | nmrsu                                                                               |
| Site                   |                                                                                     |
| Spectrometer           | spect                                                                               |
| Author                 |                                                                                     |
| Solvent                | DMSO                                                                                |
| Temperature            | 298.2                                                                               |
| Pulse                  | zgpg30                                                                              |
| Sequence               |                                                                                     |
| Number of Scans        | 3072                                                                                |
| Receiver Gain          | 2050                                                                                |
| Relaxation Delay       | 2.0000                                                                              |
| Pulse Width            | 10.0000                                                                             |
| Acquisition Time       | 1.8176                                                                              |
| Acquisition Date       | 2013-11-30T 11:48:00                                                                |
| Modification Date      | 2013-11-30T 11:48:40                                                                |
| Spectrometer Frequency | 75.47                                                                               |
| Spectral Width         | 18028.8                                                                             |
| Lowest Frequency       | -1505.1                                                                             |
| Nucleus                | 13C                                                                                 |
| Acquired Size          | 32768                                                                               |
| Spectral Size          | 65536                                                                               |

# 6-Chloro-7-(2-hydroxyphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3n).

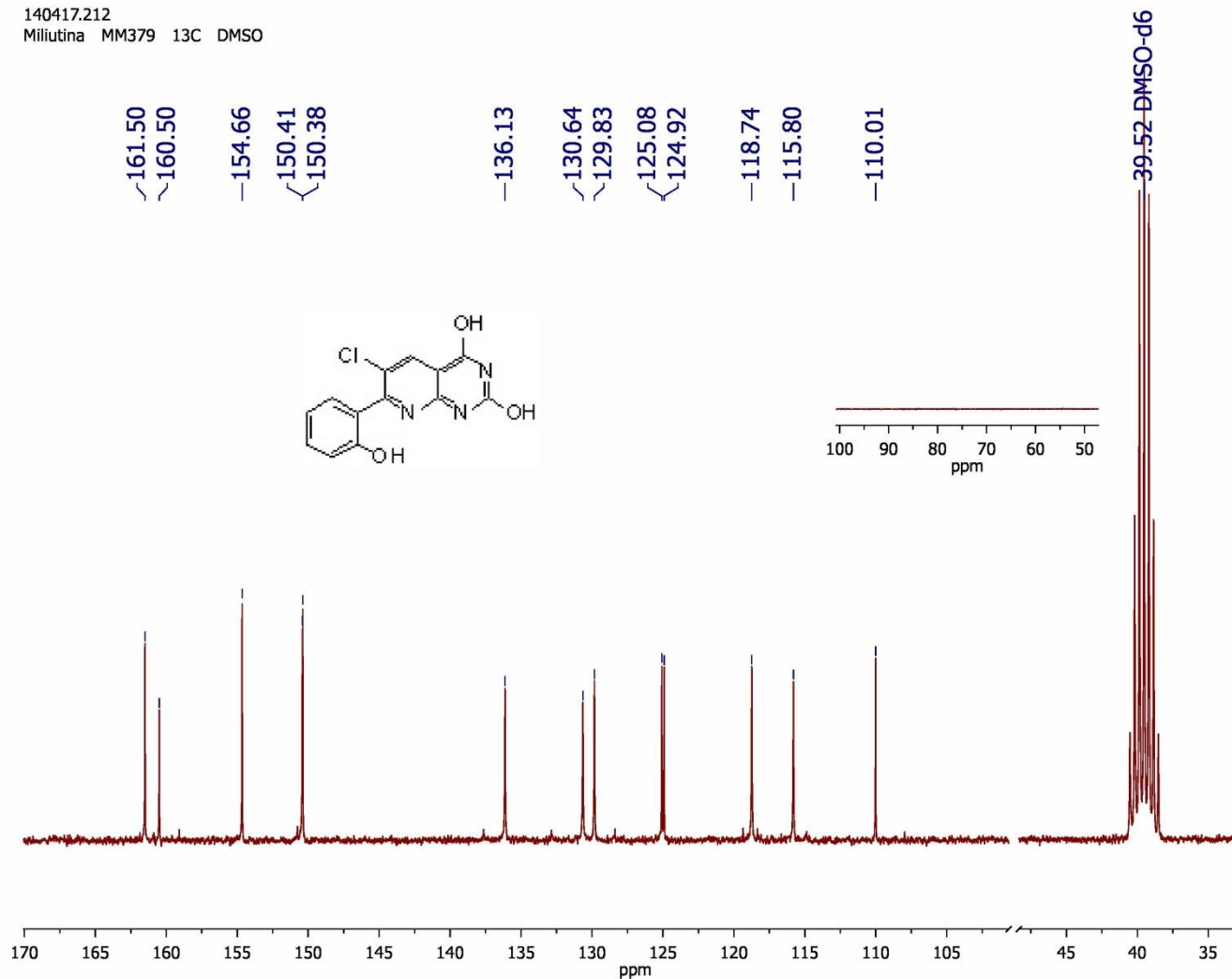
140417.212  
Millutina MM379 1H DMSO



|                        |                                                                     |
|------------------------|---------------------------------------------------------------------|
| Data File Name         | C:/Users/e/Desktop/Спектры/В/3-Cl-chromone/MM-379/140417.212/10/fid |
| Title                  | 140417.21                                                           |
| Comment                | Millutina MM379 1H DMSO                                             |
| Origin                 | Bruker BioSpin GmbH                                                 |
| Owner                  | nmr                                                                 |
| Site                   |                                                                     |
| Spectrometer           | spect                                                               |
| Author                 |                                                                     |
| Solvent                | DMSO                                                                |
| Temperature            | 298.2                                                               |
| Pulse                  | zg30                                                                |
| Sequence               |                                                                     |
| Number of Scans        | 16                                                                  |
| Receiver Gain          | 181                                                                 |
| Relaxation Delay       | 1.0000                                                              |
| Pulse Width            | 10.0000                                                             |
| Acquisition Time       | 6.3439                                                              |
| Acquisition Date       | 2014-04-17T18:02:00                                                 |
| Modification Date      | 2014-04-17T17:03:32                                                 |
| Spectrometer Frequency | 250.13                                                              |
| Spectral Width         | 5165.3                                                              |
| Lowest Frequency       | -1035.7                                                             |
| Nucleus                | 1H                                                                  |
| Acquired Size          | 32768                                                               |
| Spectral Size          | 65536                                                               |

# 6-Chloro-7-(2-hydroxyphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3n).

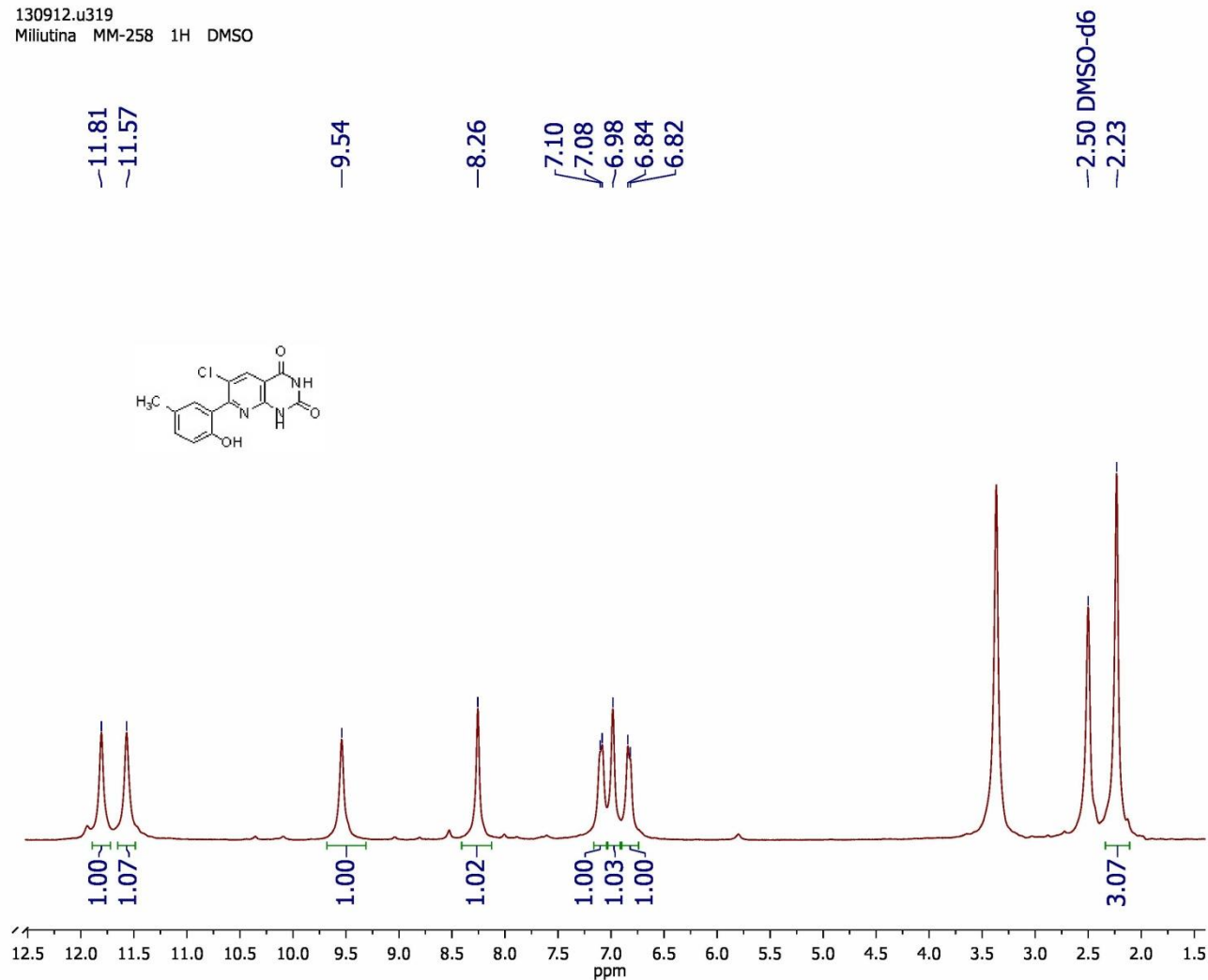
140417.212  
Millutina MM379 13C DMSO



|                        |                                                                            |
|------------------------|----------------------------------------------------------------------------|
| Data File              | C:/Users/è/Desktop/Спектры/ В/ 3-Cl- chromone/ MM-379/ 140417.212/ 11/ fid |
| Title                  | 140417.21                                                                  |
| Comment                | Millutina MM379 13C DMSO                                                   |
| Origin                 | Bruker BioSpin GmbH                                                        |
| Owner                  | nmr                                                                        |
| Site                   |                                                                            |
| Spectrometer           | spect                                                                      |
| Author                 |                                                                            |
| Solvent                | DMSO                                                                       |
| Temperature            | 298.2                                                                      |
| Pulse                  | zgpg30                                                                     |
| Sequence               |                                                                            |
| Number of Scans        | 1024                                                                       |
| Receiver Gain          | 2050                                                                       |
| Relaxation Delay       | 2.0000                                                                     |
| Pulse Width            | 10.0000                                                                    |
| Acquisition Time       | 2.1846                                                                     |
| Acquisition Date       | 2014-04-17T 19:16:00                                                       |
| Modification Date      | 2014-04-17T 18:17:36                                                       |
| Spectrometer Frequency | 62.90                                                                      |
| Spectral Width         | 15000.0                                                                    |
| Lowest Frequency       | -1235.2                                                                    |
| Nucleus                | 13C                                                                        |
| Acquired Size          | 32768                                                                      |
| Spectral Size          | 65536                                                                      |

**6-Chloro-7-(2-hydroxy-5-methylphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3o).**

130912.u319  
Miljutina MM-258 1H DMSO



Data File Name C:/Users/è/  
Desktop/  
Спектры/ В/  
3-Cl-  
chromone/  
MM-258/  
130912.u319/  
10/ fid

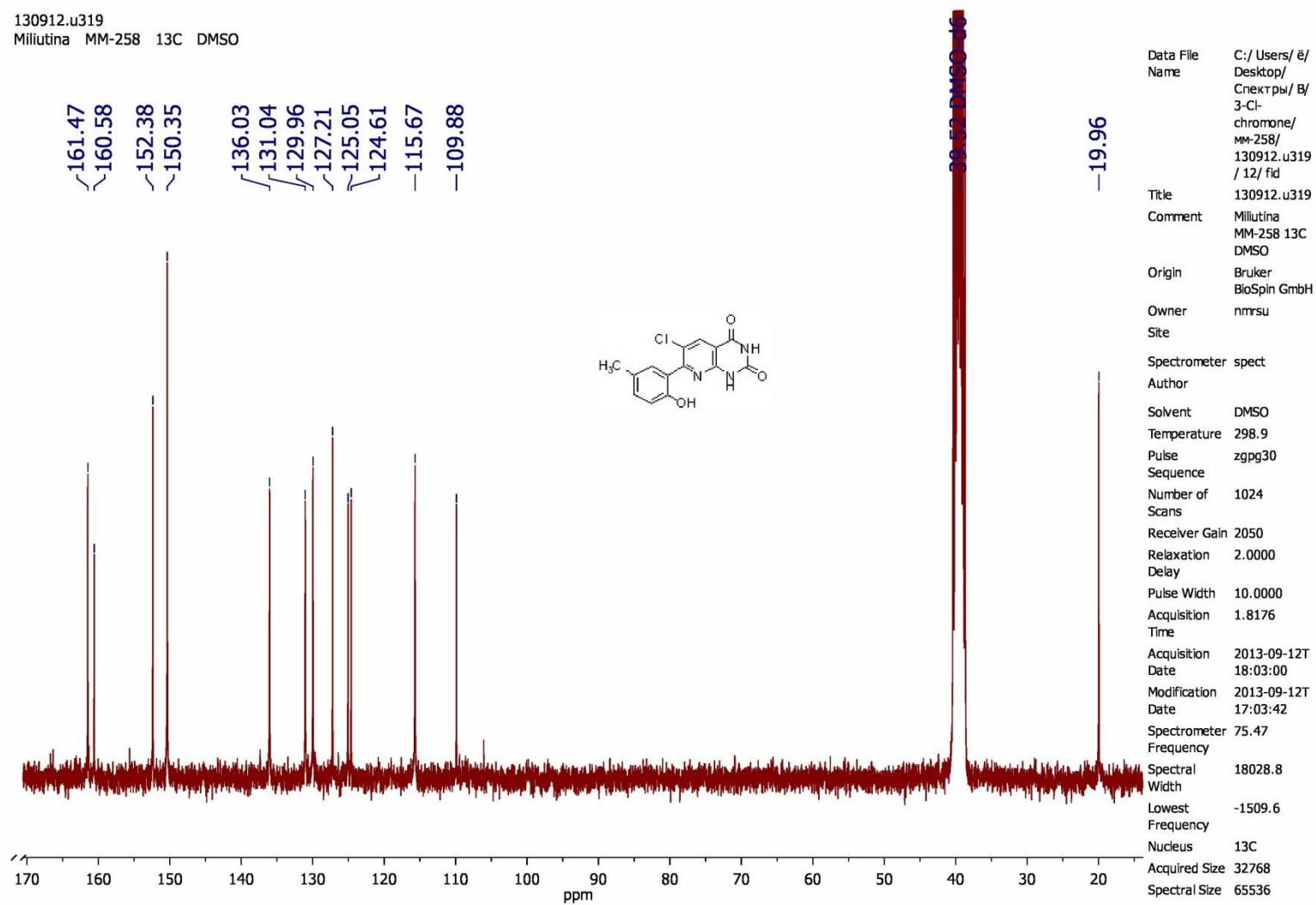
Title 130912.u319  
Comment Miljutina  
MM-258 1H  
DMSO  
Origin Bruker BioSpin  
GmbH  
Owner nmrsu  
Site

Spectrometer spect  
Author

Solvent DMSO  
Temperature 298.2  
Pulse Sequence zg30  
Number of Scans 16  
Receiver Gain 90  
Relaxation Delay 1.0000  
Pulse Width 10.0000  
Acquisition Time 5.2954  
Acquisition Date 2013-09-12T1  
5:09:00  
Modification Date 2013-09-12T1  
4:09:36  
Spectrometer Frequency 300.13  
Spectral Width 6188.1  
Lowest Frequency -1288.1  
Nucleus 1H  
Acquired Size 32768  
Spectral Size 65536

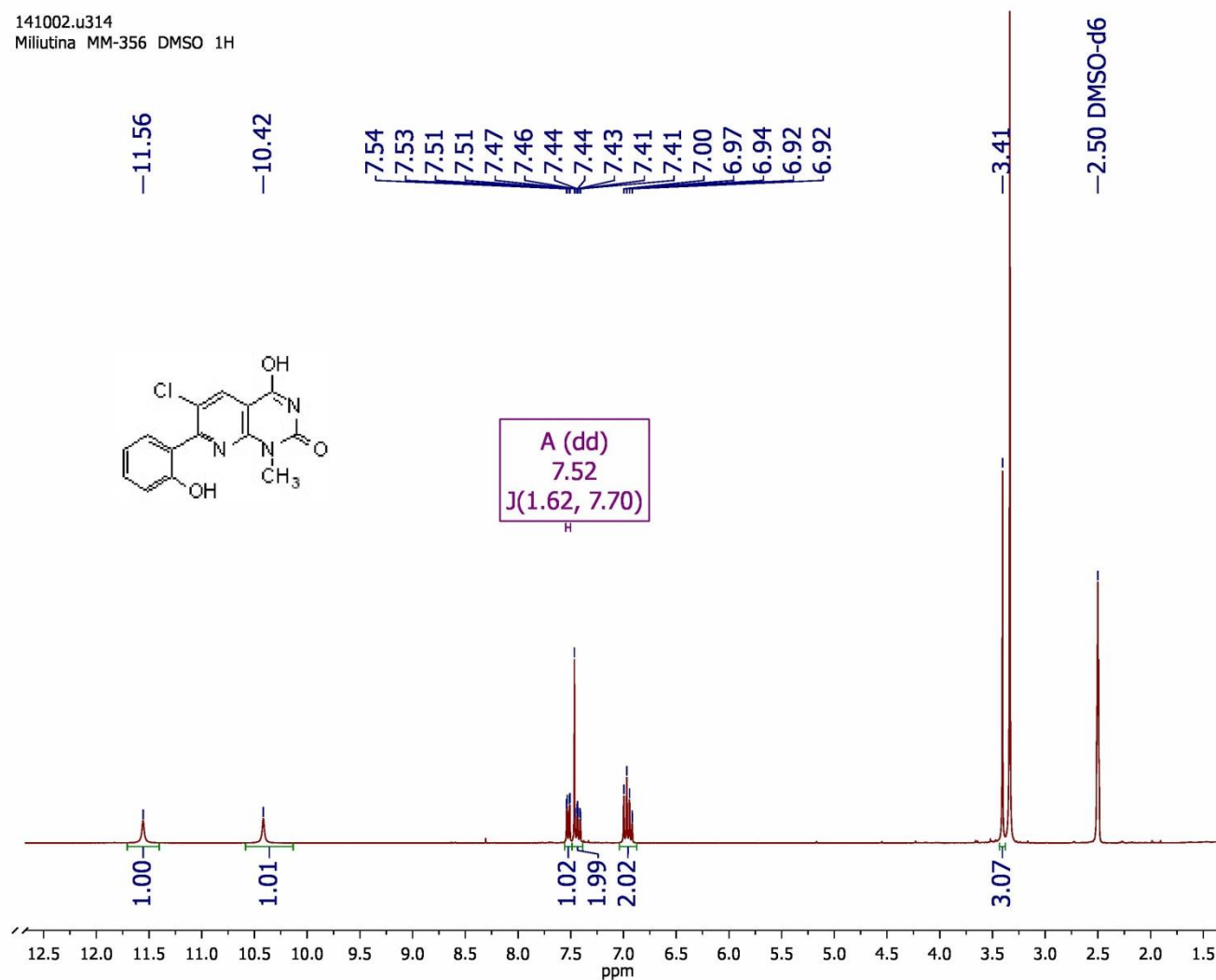
**6-Chloro-7-(2-hydroxy-5-methylphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3o).**

130912.u319  
Millutina MM-258 13C DMSO



**6-Chloro-7-(2-hydroxyphenyl)-1-methylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3p).**

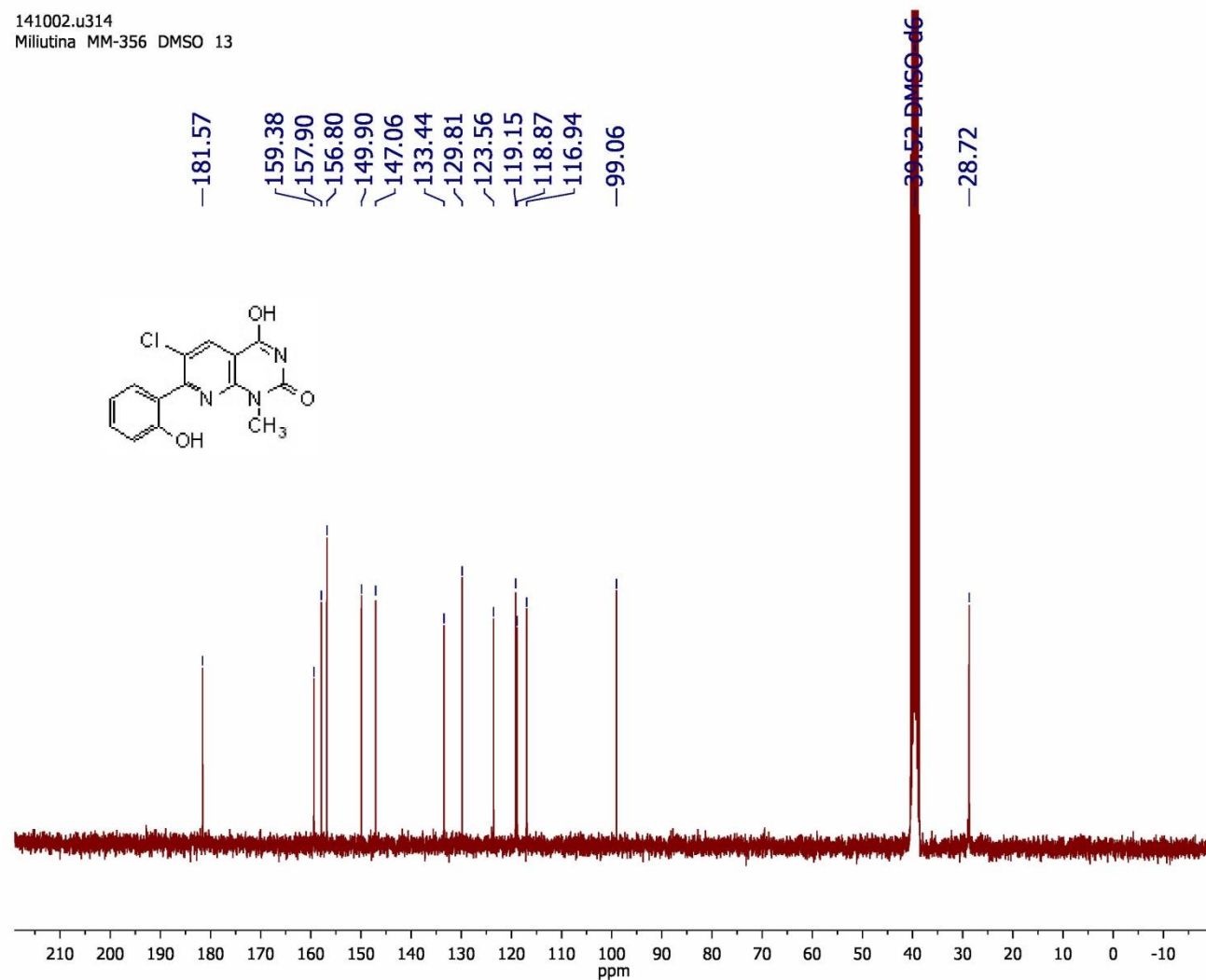
141002.u314  
Miliutina MM-356 DMSO 1H



|                        |                                                                          |
|------------------------|--------------------------------------------------------------------------|
| Data File Name         | C:/Users/é/Desktop/Спектры/ C/3-Cl-chromone/MM-356/141002.u314 / 10/ fid |
| Title                  | 141002.u314                                                              |
| Comment                | Miliutina MM-356 DMSO 1H                                                 |
| Origin                 | Bruker BioSpin GmbH                                                      |
| Owner                  | nmrsu                                                                    |
| Site                   |                                                                          |
| Spectrometer           | spect                                                                    |
| Author                 |                                                                          |
| Solvent                | DMSO                                                                     |
| Temperature            | 298.2                                                                    |
| Pulse Sequence         | zg30                                                                     |
| Number of Scans        | 16                                                                       |
| Receiver Gain          | 144                                                                      |
| Relaxation Delay       | 1.0000                                                                   |
| Pulse Width            | 10.0000                                                                  |
| Acquisition Time       | 5.2954                                                                   |
| Acquisition Date       | 2014-10-02T 13:18:00                                                     |
| Modification Date      | 2014-10-02T 12:18:22                                                     |
| Spectrometer Frequency | 300.13                                                                   |
| Spectral Width         | 6188.1                                                                   |
| Lowest Frequency       | -1242.0                                                                  |
| Nucleus                | 1H                                                                       |
| Acquired Size          | 32768                                                                    |
| Spectral Size          | 65536                                                                    |

**6-Chloro-7-(2-hydroxyphenyl)-1-methylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (3p).**

141002.u314  
Miliutina MM-356 DMSO 13

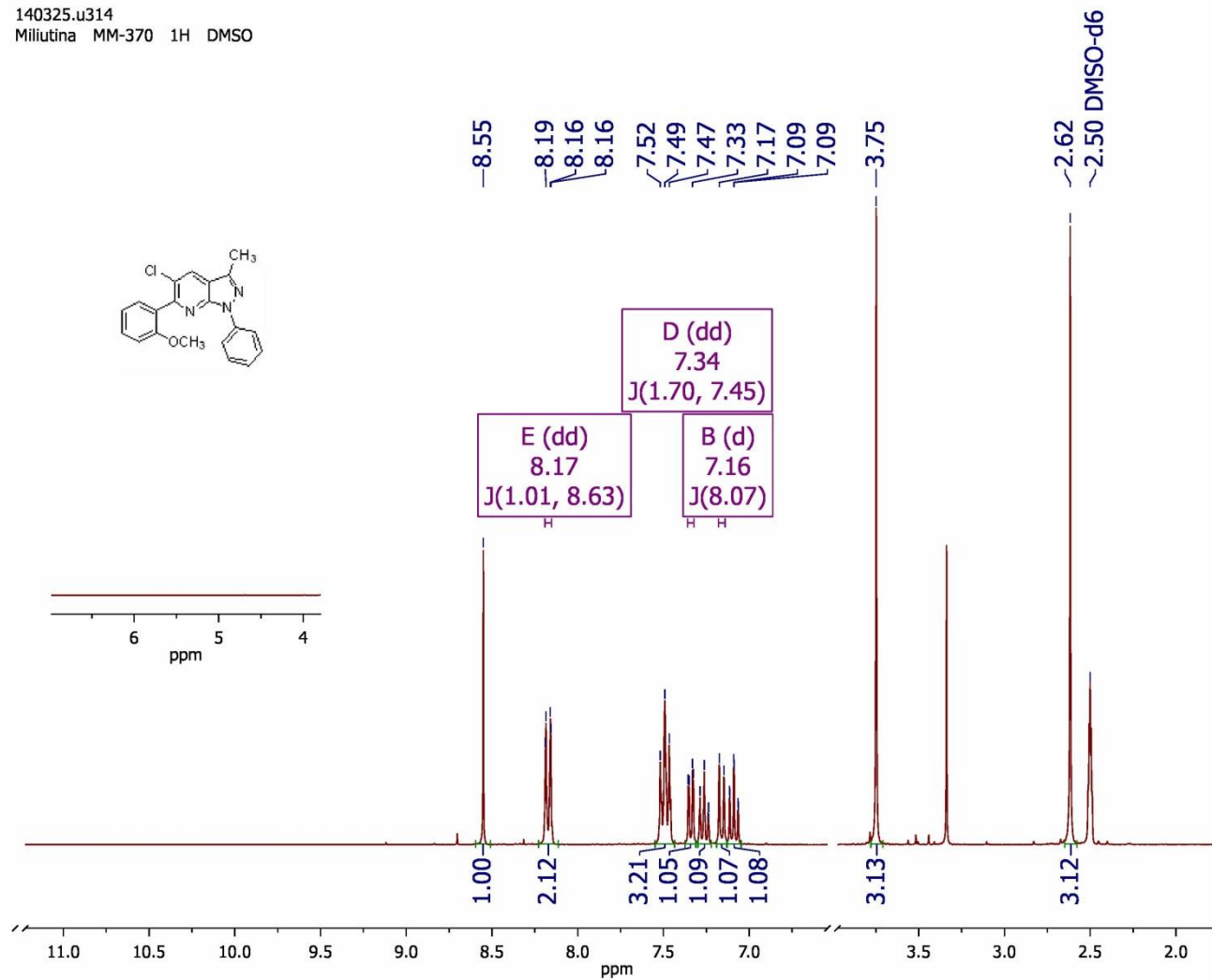


|                        |                                                                           |
|------------------------|---------------------------------------------------------------------------|
| Data File Name         | C:/Users/ě/Desktop/Спектры/ C/3-Cl-chromone/ MM-356/ 141002.u314/ 11/ Fid |
| Title                  | 141002.u314                                                               |
| Comment                | Miliutina MM-356 DMSO 13                                                  |
| Origin                 | Bruker BioSpin GmbH                                                       |
| Owner                  | nmrsu                                                                     |
| Site                   |                                                                           |
| Spectrometer           | spect                                                                     |
| Author                 |                                                                           |
| Solvent                | DMSO                                                                      |
| Temperature            | 298.2                                                                     |
| Pulse                  | zgpg30                                                                    |
| Sequence               |                                                                           |
| Number of Scans        | 3072                                                                      |
| Receiver Gain          | 2050                                                                      |
| Relaxation             | 2.0000                                                                    |
| Delay                  |                                                                           |
| Pulse Width            | 10.0000                                                                   |
| Acquisition Time       | 1.8176                                                                    |
| Acquisition Date       | 2014-10-04T21:35:00                                                       |
| Modification Date      | 2014-10-04T20:35:16                                                       |
| Spectrometer Frequency | 75.47                                                                     |
| Spectral Width         | 18028.8                                                                   |
| Lowest Frequency       | -1502.5                                                                   |
| Nucleus                | 13C                                                                       |
| Acquired Size          | 32768                                                                     |
| Spectral Size          | 65536                                                                     |

# 5-Chloro-6-(2-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine (3q).

140325.u314

Millutina MM-370 1H DMSO



Data File Name: C:/Users/è/Desktop/Спектры/В/3-Cl-chromone/мм-370/140325.u314 / 10/ fid

Title: 140325.u314

Comment: Millutina MM-370 1H DMSO

Origin: Bruker BioSpin GmbH

Owner: nmrsu

Site:

Spectrometer: spect

Author:

Solvent: DMSO

Temperature: 298.2

Pulse Sequence: zg30

Number of Scans: 16

Receiver Gain: 90

Relaxation Delay: 1.0000

Pulse Width: 10.0000

Acquisition Time: 5.2954

Acquisition Date: 2014-03-25T15:26:00

Modification Date: 2014-03-25T15:26:40

Spectrometer Frequency: 300.13

Spectral Width: 6188.1

Lowest Frequency: -1253.2

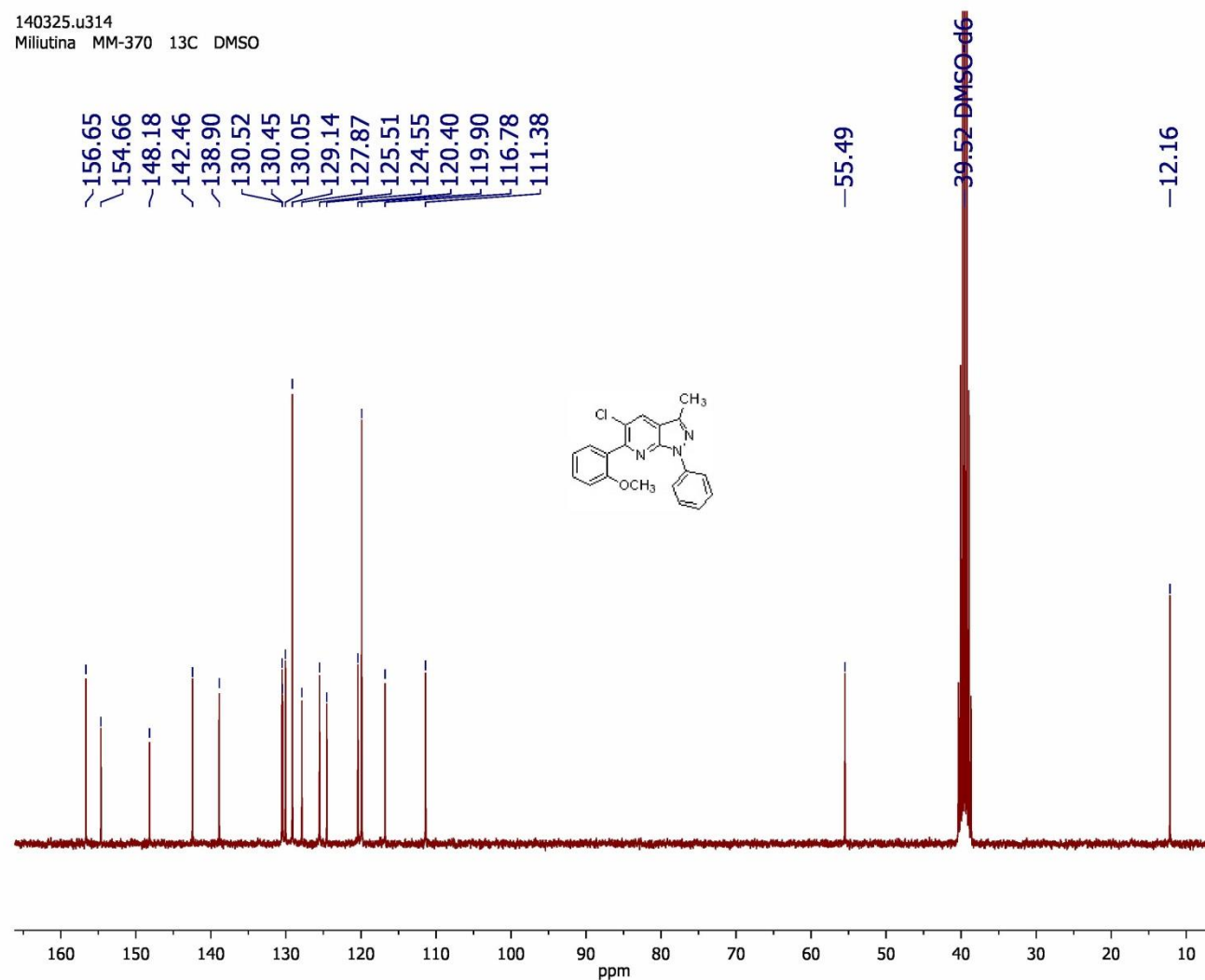
Nucleus: 1H

Acquired Size: 32768

Spectral Size: 65536

# 5-Chloro-6-(2-methoxyphenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine (3q).

140325.u314  
Miljutina MM-370 13C DMSO



Data File Name C:/Users/ë/Desktop/Спектры/ B/ 3-Cl- chromone/ MM-370/ 140325.u314/ 11/ fid

Title 140325.u314

Comment Miljutina MM-370 13C DMSO

Origin Bruker BioSpin GmbH

Owner nmrsu

Site

Spectrometer spect

Author

Solvent DMSO

Temperature 298.2

Pulse zgpg30

Sequence

Number of Scans 1024

Receiver Gain 2050

Relaxation Delay 2.0000

Pulse Width 10.0000

Acquisition Time 1.8176

Acquisition Date 2014-03-25T2 1:06:00

Modification Date 2014-03-25T2 1:06:14

Spectrometer Frequency 75.47

Spectral Width 18028.8

Lowest Frequency -1507.5

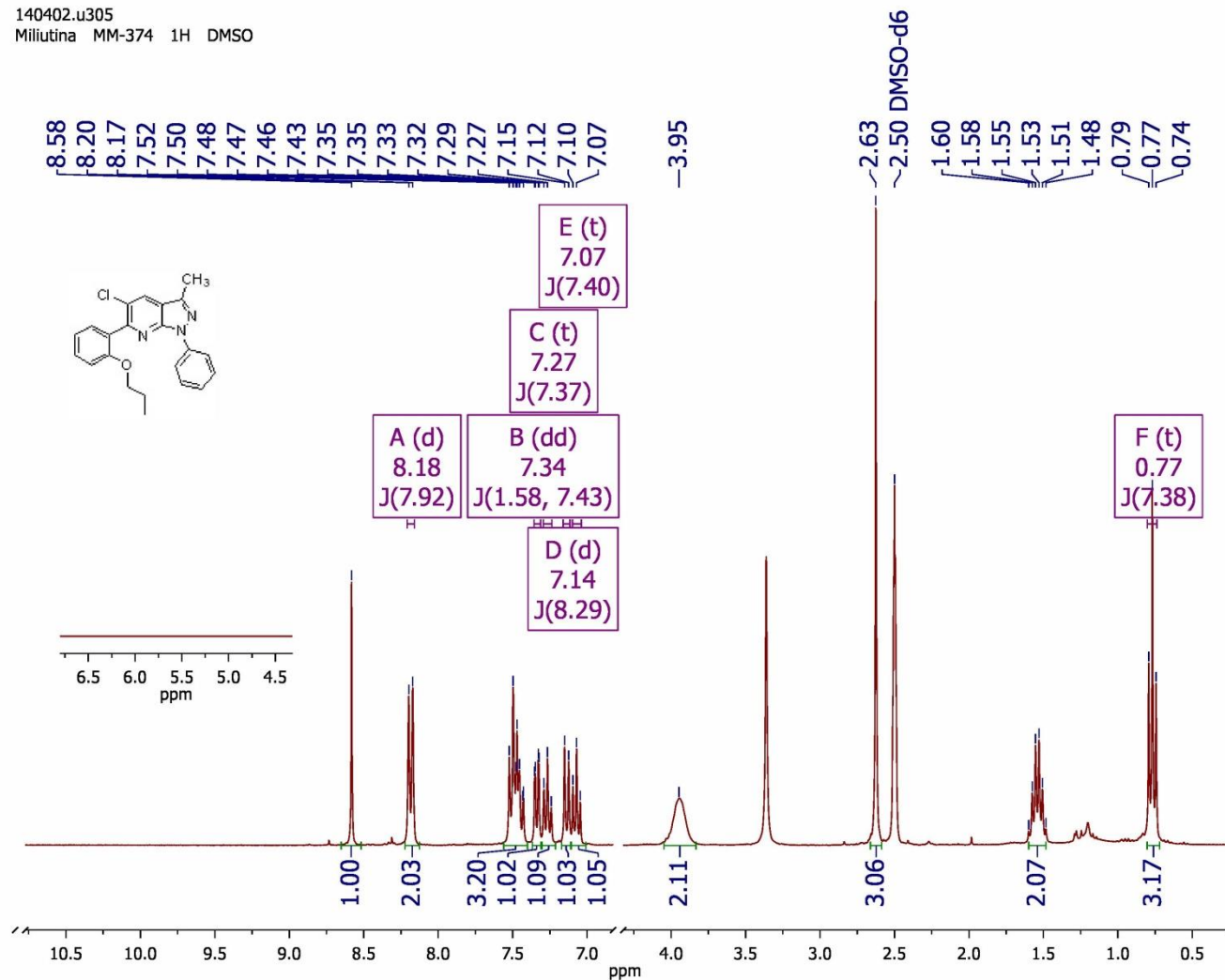
Nucleus 13C

Acquired Size 32768

Spectral Size 65536

# 5-Chloro-3-methyl-1-phenyl-6-(2-propoxyphenyl)-1H-pyrazolo[3,4-*b*]pyridine (3r).

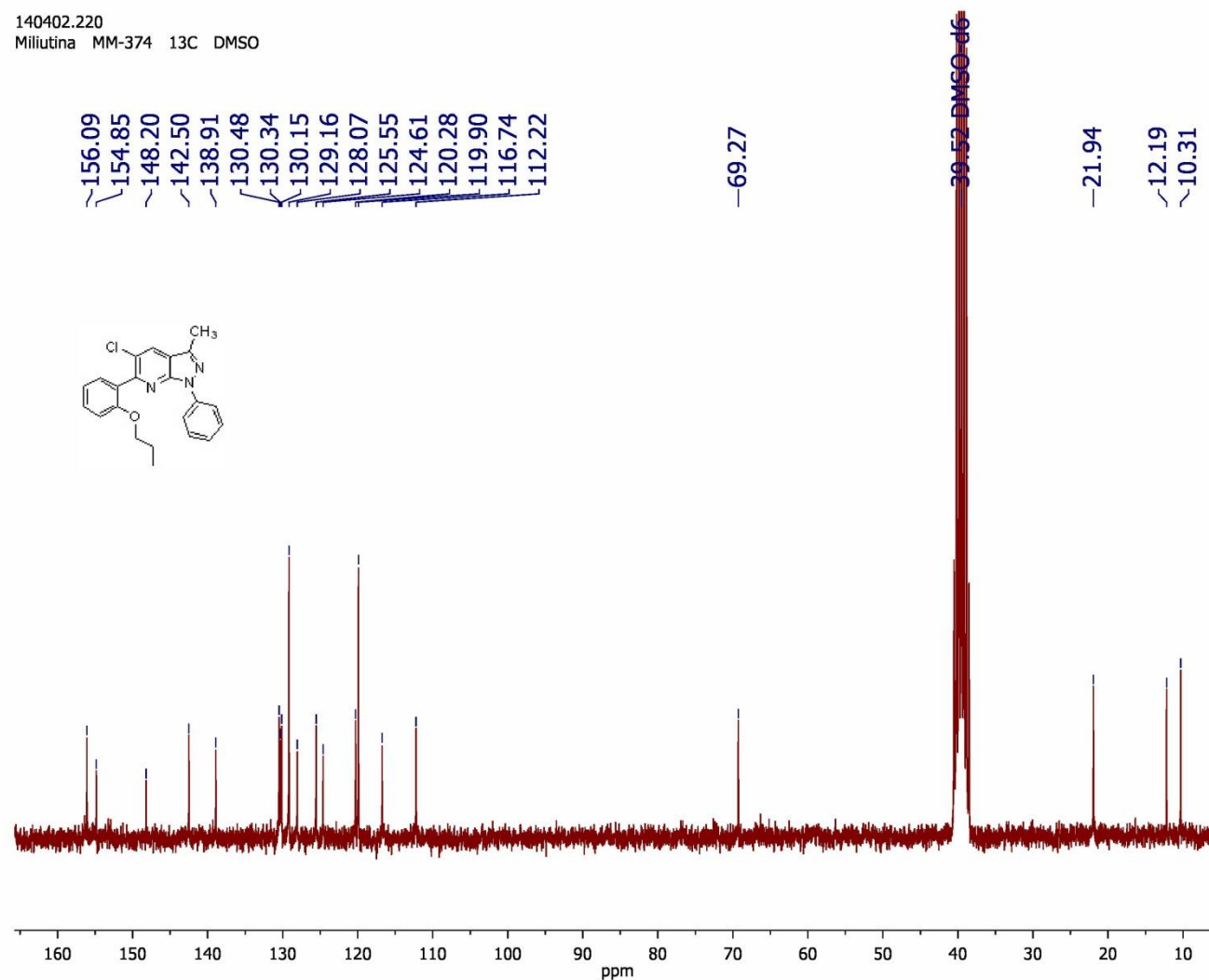
140402.u305  
Miliutina MM-374 1H DMSO



|                        |                                                                       |
|------------------------|-----------------------------------------------------------------------|
| Data File Name         | C:/Users/è/Desktop/Спектры/В/3-Cl-chromone/MM-374/140402.u305/10/ fid |
| Title                  | 140402.u305                                                           |
| Comment                | Miliutina MM-374 1H DMSO                                              |
| Origin                 | Bruker BioSpin GmbH                                                   |
| Owner                  | nmrsu                                                                 |
| Site                   |                                                                       |
| Spectrometer           | spect                                                                 |
| Author                 |                                                                       |
| Solvent                | DMSO                                                                  |
| Temperature            | 298.2                                                                 |
| Pulse Sequence         | zg30                                                                  |
| Number of Scans        | 16                                                                    |
| Receiver Gain          | 101                                                                   |
| Relaxation Delay       | 1.0000                                                                |
| Pulse Width            | 10.0000                                                               |
| Acquisition Time       | 5.2954                                                                |
| Acquisition Date       | 2014-04-02T09:25:00                                                   |
| Modification Date      | 2014-04-02T08:25:12                                                   |
| Spectrometer Frequency | 300.13                                                                |
| Spectral Width         | 6188.1                                                                |
| Lowest Frequency       | -1255.0                                                               |
| Nucleus                | 1H                                                                    |
| Acquired Size          | 32768                                                                 |
| Spectral Size          | 65536                                                                 |

# 5-Chloro-3-methyl-1-phenyl-6-(2-propoxyphenyl)-1H-pyrazolo[3,4-*b*]pyridine (3r).

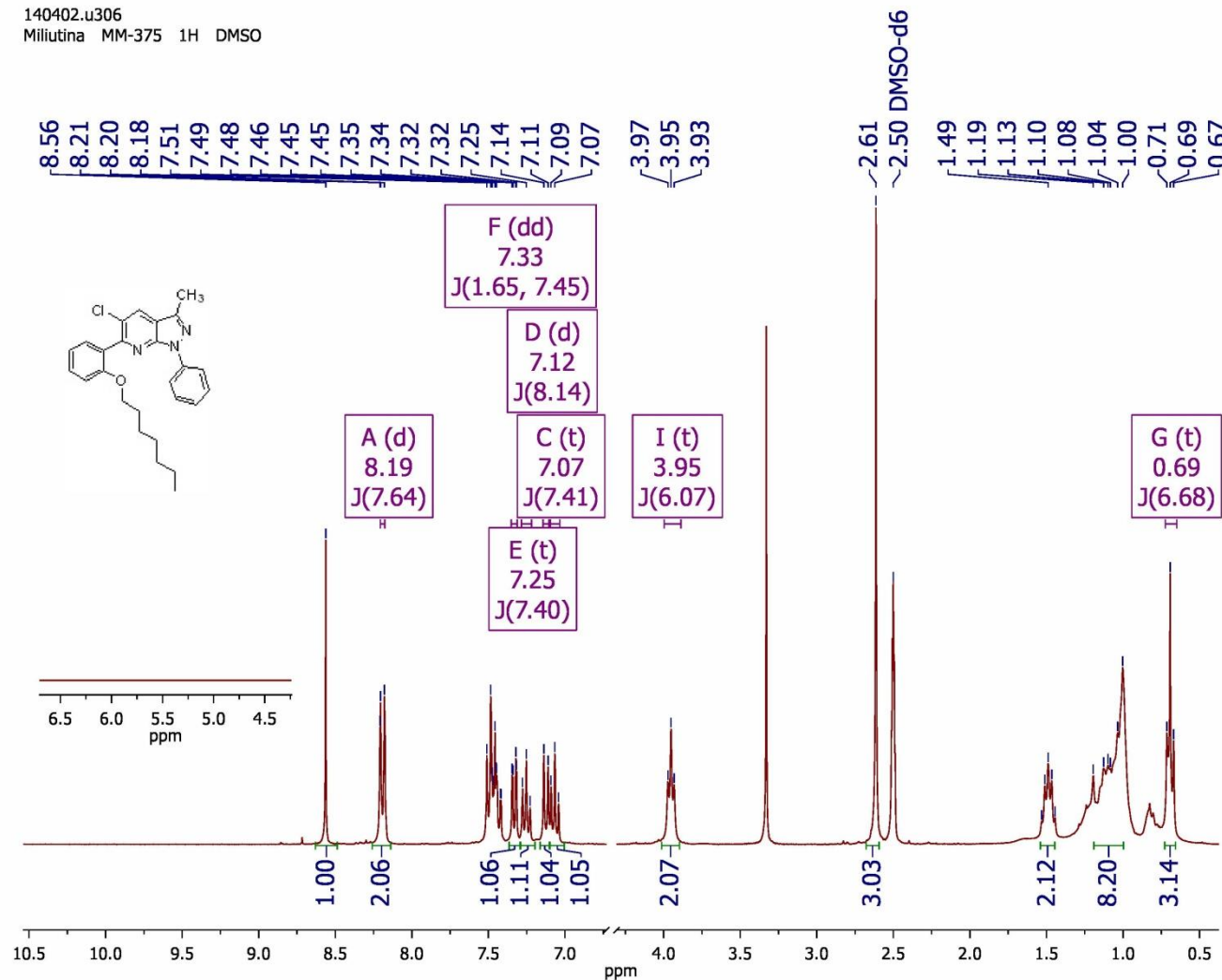
140402.220  
Millutina MM-374 13C DMSO



|                        |                                                                            |
|------------------------|----------------------------------------------------------------------------|
| Data File Name         | C:/Users/è/Desktop/Спектры/ B/ 3-Cl- chromone/ MM-374/ 140402.220/ 10/ fid |
| Title                  | 140402.22                                                                  |
| Comment                | Millutina MM-374 13C DMSO                                                  |
| Origin                 | Bruker BioSpin GmbH                                                        |
| Owner                  | nmr                                                                        |
| Site                   |                                                                            |
| Spectrometer           | spect                                                                      |
| Author                 |                                                                            |
| Solvent                | DMSO                                                                       |
| Temperature            | 298.0                                                                      |
| Pulse                  | zgpg30                                                                     |
| Sequence               |                                                                            |
| Number of Scans        | 1024                                                                       |
| Receiver Gain          | 2050                                                                       |
| Relaxation Delay       | 2.0000                                                                     |
| Pulse Width            | 10.0000                                                                    |
| Acquisition Time       | 2.1846                                                                     |
| Acquisition Date       | 2014-04-02T 15:21:00                                                       |
| Modification Date      | 2014-04-02T 14:22:02                                                       |
| Spectrometer Frequency | 62.90                                                                      |
| Spectral Width         | 15000.0                                                                    |
| Lowest Frequency       | -1240.3                                                                    |
| Nucleus                | 13C                                                                        |
| Acquired Size          | 32768                                                                      |
| Spectral Size          | 65536                                                                      |

# 5-Chloro-6-(2-(heptyloxy)phenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-*b*]pyridine (3s).

140402.u306  
Millutina MM-375 1H DMSO



Data File Name: C:/Users/ë/Desktop/Спектры/ B/ 3-Cl- chromone/ MM-375/ 140402.u306/ 10/ fid

Title: 140402.u306

Comment: Millutina MM-375 1H DMSO

Origin: Bruker BioSpin GmbH

Owner: nmrsu

Site:

Spectrometer: spect

Author:

Solvent: DMSO

Temperature: 298.2

Pulse: zg30

Sequence:

Number of Scans: 16

Receiver Gain: 51

Relaxation Delay: 1.0000

Pulse Width: 10.0000

Acquisition Time: 5.2954

Acquisition Date: 2014-04-02T09:29:00

Modification Date: 2014-04-02T08:29:48

Spectrometer Frequency: 300.13

Spectral Width: 6188.1

Lowest Frequency: -1255.3

Nucleus: 1H

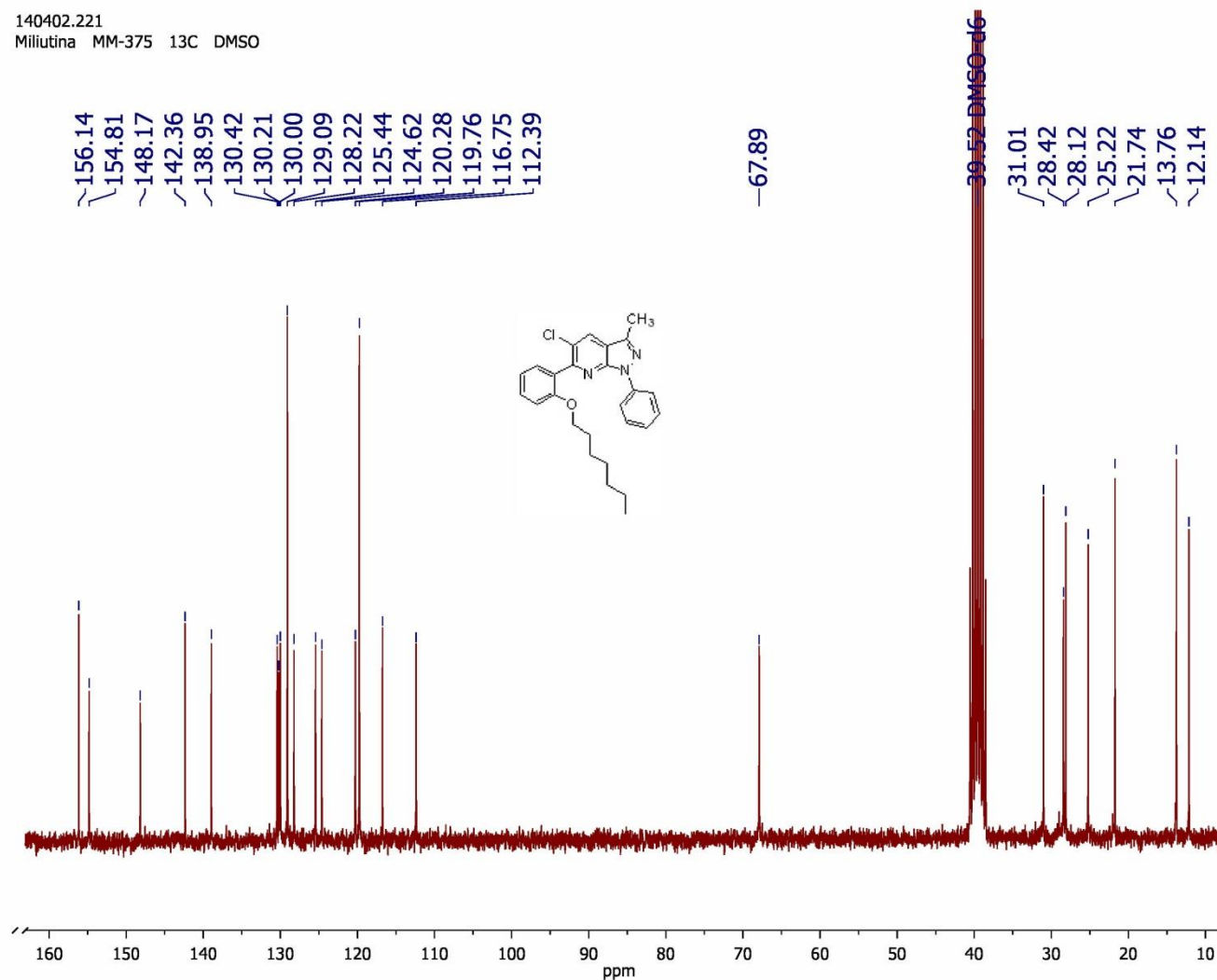
Acquired Size: 32768

Spectral Size: 65536

# 5-Chloro-6-(2-(heptyloxy)phenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-*b*]pyridine (3s).

140402.221

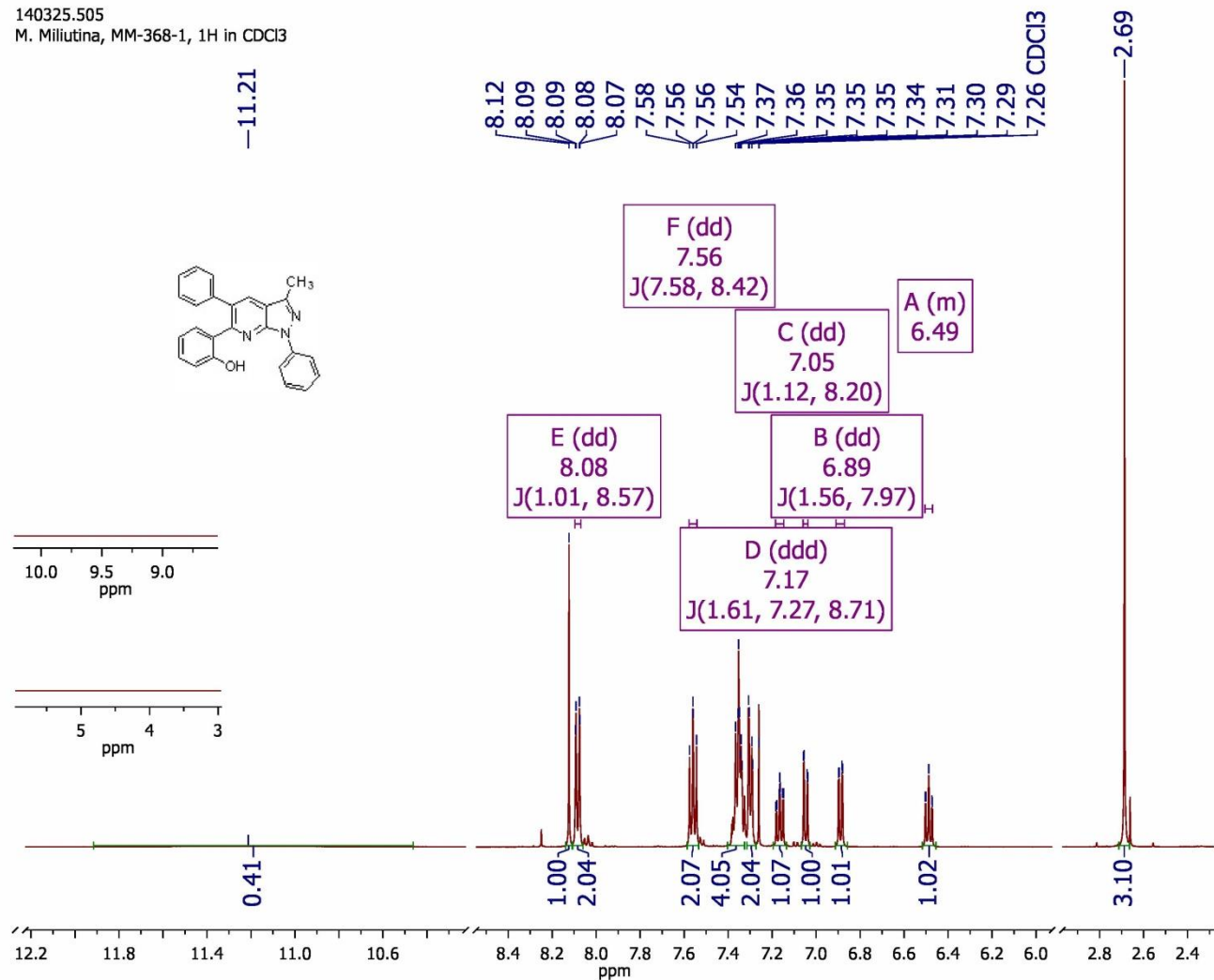
Millutina MM-375 13C DMSO



|                        |                                                                            |
|------------------------|----------------------------------------------------------------------------|
| Data File Name         | C:/Users/è/Desktop/Спектры/ В/ 3-Cl- chromone/ MM-375/ 140402.221/ 10/ fid |
| Title                  | 140402.22                                                                  |
| Comment                | Millutina MM-375 13C DMSO                                                  |
| Origin                 | Bruker BioSpin GmbH                                                        |
| Owner                  | nmr                                                                        |
| Site                   |                                                                            |
| Spectrometer           | spect                                                                      |
| Author                 |                                                                            |
| Solvent                | DMSO                                                                       |
| Temperature            | 298.1                                                                      |
| Pulse Sequence         | zgpg30                                                                     |
| Number of Scans        | 1024                                                                       |
| Receiver Gain          | 2050                                                                       |
| Relaxation Delay       | 2.0000                                                                     |
| Pulse Width            | 10.0000                                                                    |
| Acquisition Time       | 2.1846                                                                     |
| Acquisition Date       | 2014-04-02T1 7:01:00                                                       |
| Modification Date      | 2014-04-02T1 6:01:38                                                       |
| Spectrometer Frequency | 62.90                                                                      |
| Spectral Width         | 15000.0                                                                    |
| Lowest Frequency       | -1240.7                                                                    |
| Nucleus                | 13C                                                                        |
| Acquired Size          | 32768                                                                      |
| Spectral Size          | 65536                                                                      |

## 2-(3-Methyl-1,5-diphenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (3t).

140325.505  
M. Miljutina, MM-368-1, 1H in CDCl<sub>3</sub>



Data File Name C:/Users/ë/Desktop/Спектры/ B/ 3-Cl-chromone/ MM-368/ 368-1/ 140325.505/ 10/ fid

Title 140325.51

Comment M. Miljutina, MM-368-1, 1H in CDCl<sub>3</sub>

Origin Bruker BioSpin GmbH

Owner Administrator

Site

Spectrometer spect

Author

Solvent CDCl<sub>3</sub>

Temperature 300.0

Pulse Sequence zg30

Number of Scans 32

Receiver Gain 128

Relaxation 1.0000

Delay

Pulse Width 9.8000

Acquisition Time 3.1720

Acquisition Date 2014-03-25T19:46:00

Modification Date 2014-03-25T19:47:02

Spectrometer 500.13

Frequency

Spectral Width 10330.6

Lowest Frequency -2089.5

Nucleus 1H

Acquired Size 32768

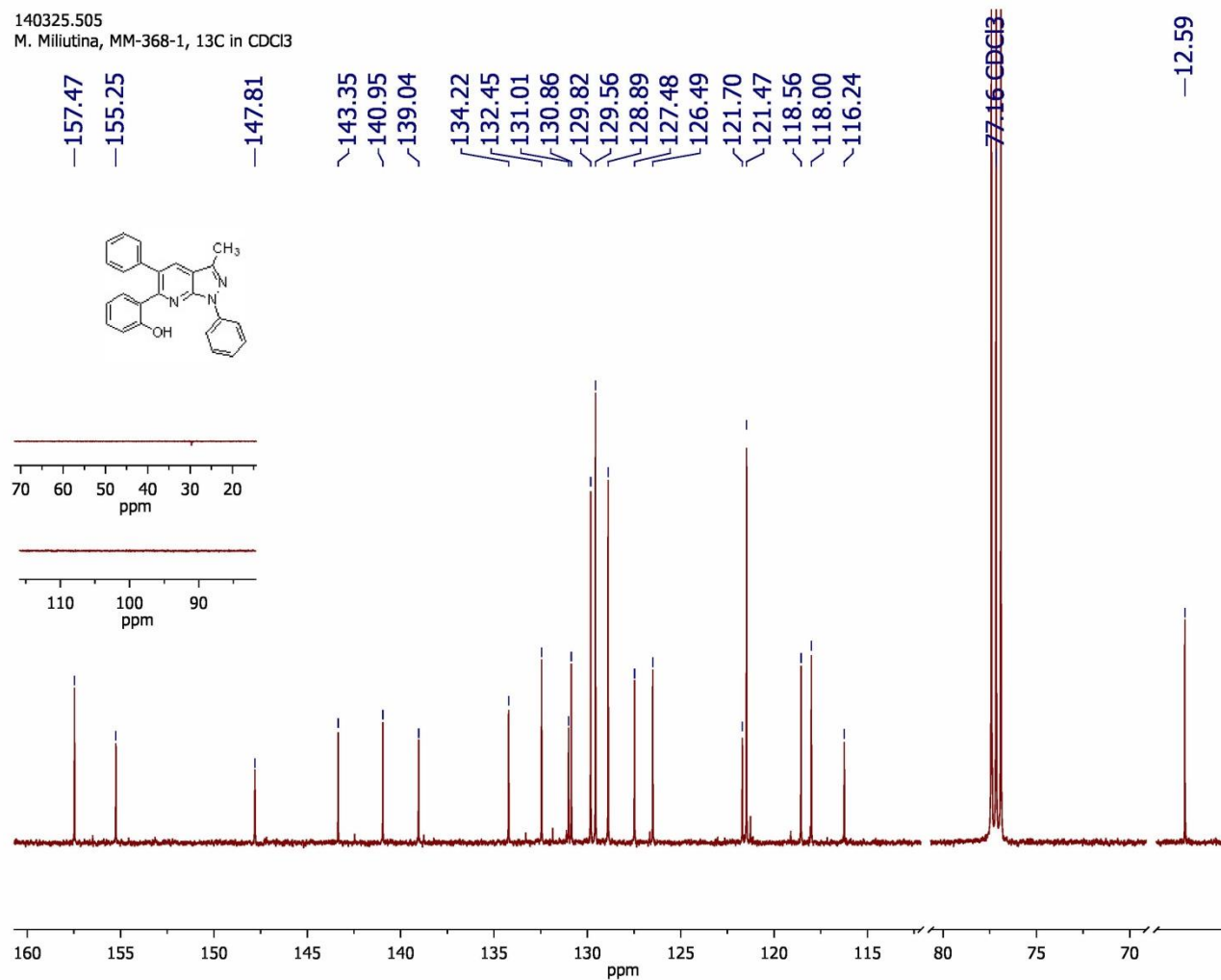
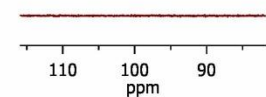
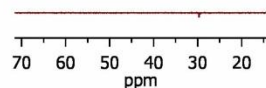
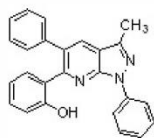
Spectral Size 65536

## 2-(3-Methyl-1,5-diphenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (3t).

140325.505

M. Miliutina, MM-368-1, <sup>13</sup>C in CDCl<sub>3</sub>

157.47 155.25 147.81 143.35 140.95 139.04 134.22 132.45 131.01 130.86 129.82 129.56 128.89 127.48 126.49 121.70 121.47 118.56 118.00 116.24



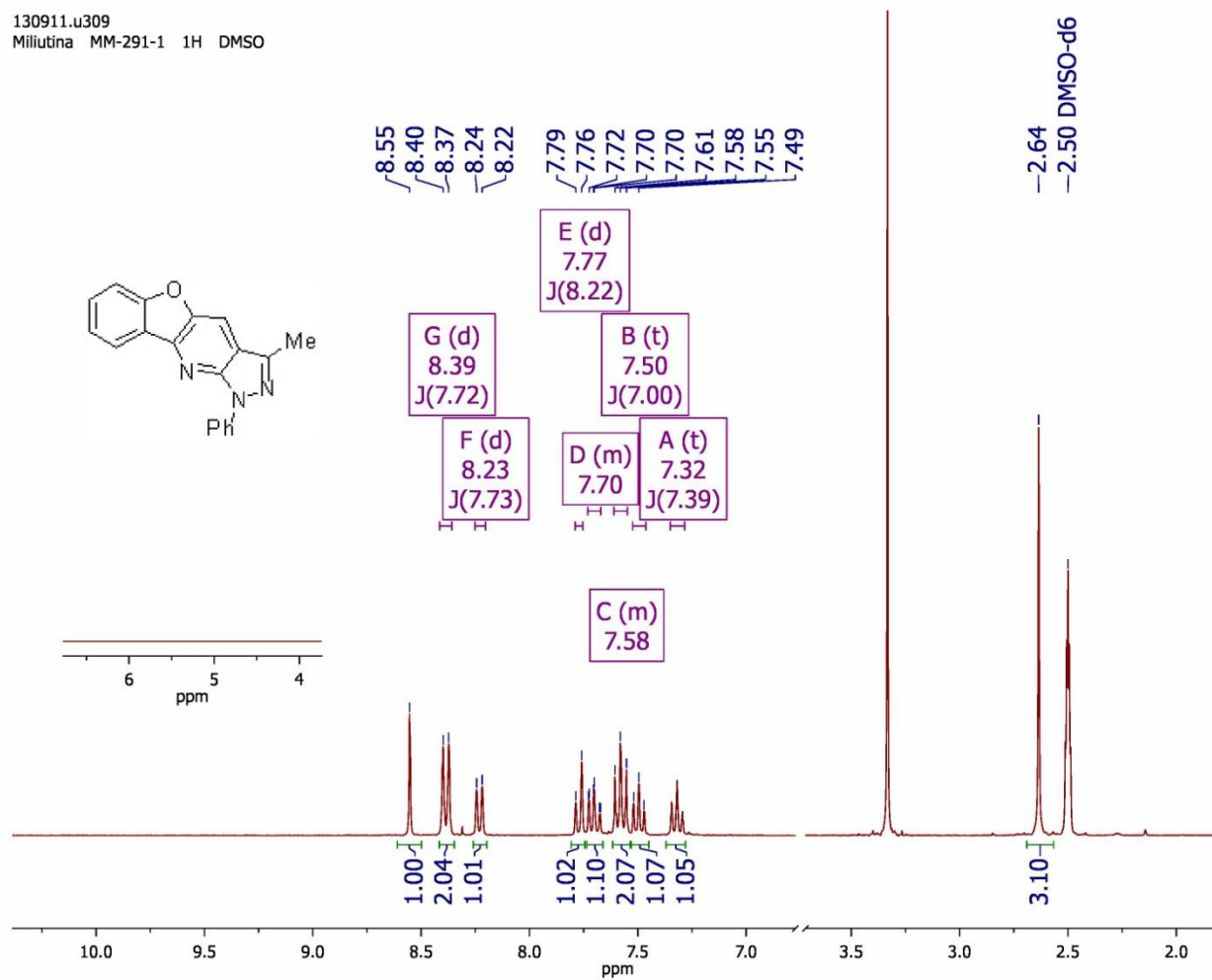
12.59

|                        |                                                                                   |
|------------------------|-----------------------------------------------------------------------------------|
| Data File Name         | C:/Users/ě/Desktop/Спектры/ В/ 3-Cl- chromone/ mm-368/ 368-1/ 140325.505/ 15/ fid |
| Title                  | 140325.51                                                                         |
| Comment                | M. Miliutina, MM-368-1, <sup>13</sup> C in CDCl <sub>3</sub>                      |
| Origin                 | Bruker BioSpin GmbH                                                               |
| Owner                  | Administrator                                                                     |
| Site                   |                                                                                   |
| Spectrometer           | spect                                                                             |
| Author                 |                                                                                   |
| Solvent                | CDCl <sub>3</sub>                                                                 |
| Temperature            | 300.0                                                                             |
| Pulse                  | zgpg30                                                                            |
| Sequence               |                                                                                   |
| Number of Scans        | 2048                                                                              |
| Receiver Gain          | 20642                                                                             |
| Relaxation Delay       | 2.0000                                                                            |
| Pulse Width            | 9.0000                                                                            |
| Acquisition Time       | 1.0912                                                                            |
| Acquisition Date       | 2014-03-26T03:32:00                                                               |
| Modification Date      | 2014-03-26T03:32:34                                                               |
| Spectrometer Frequency | 125.76                                                                            |
| Spectral Width         | 30030.0                                                                           |
| Lowest Frequency       | -2423.0                                                                           |
| Nucleus                | <sup>13</sup> C                                                                   |
| Acquired Size          | 32768                                                                             |
| Spectral Size          | 65536                                                                             |

# **<sup>1</sup>H and <sup>13</sup>C NMR spectra of products 4.**

## **3-Methyl-1-phenyl-1H-benzofuro[3,2-b]pyrazolo[4,3-e]pyridine (4a).**

130911.u309  
Miliutina MM-291-1 1H DMSO



Data File Name: C:/Users/ē/Desktop/Спектры/ B/ 3-Cl- chromone/ MM-291/ 130911.u309/ 10/ pdata/ 1/ 1r

Title: 130911.u309

Comment: Miliutina MM-291-1 1H DMSO

Origin: Bruker BioSpin GmbH

Owner: nmrsu

Site: spect

Spectrometer: spect

Author: spect

Solvent: DMSO

Temperature: 298.2

Pulse Sequence: zg30

Number of Scans: 16

Receiver Gain: 114

Relaxation Delay: 1.0000

Pulse Width: 10.0000

Acquisition Time: 5.2954

Acquisition Date: 2013-09-11T09:32:00

Modification Date: 2013-09-11T08:32:52

Spectrometer Frequency: 300.13

Spectral Width: 6188.1

Lowest Frequency: -1253.2

Nucleus: 1H

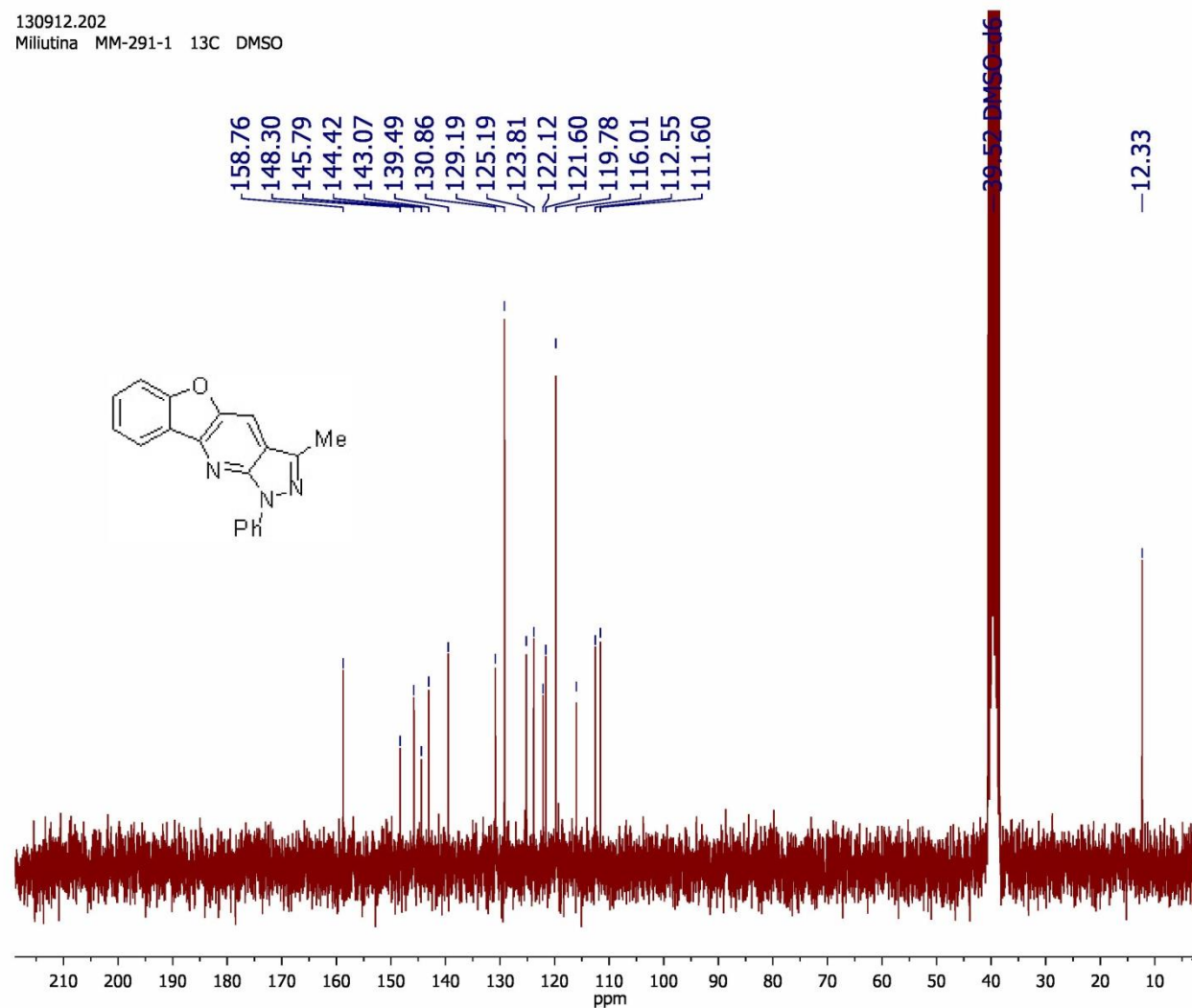
Acquired Size: 32768

Spectral Size: 32768

### 3-Methyl-1-phenyl-1H-benzofuro[3,2-b]pyrazolo[4,3-e]pyridine (4a).

130912.202

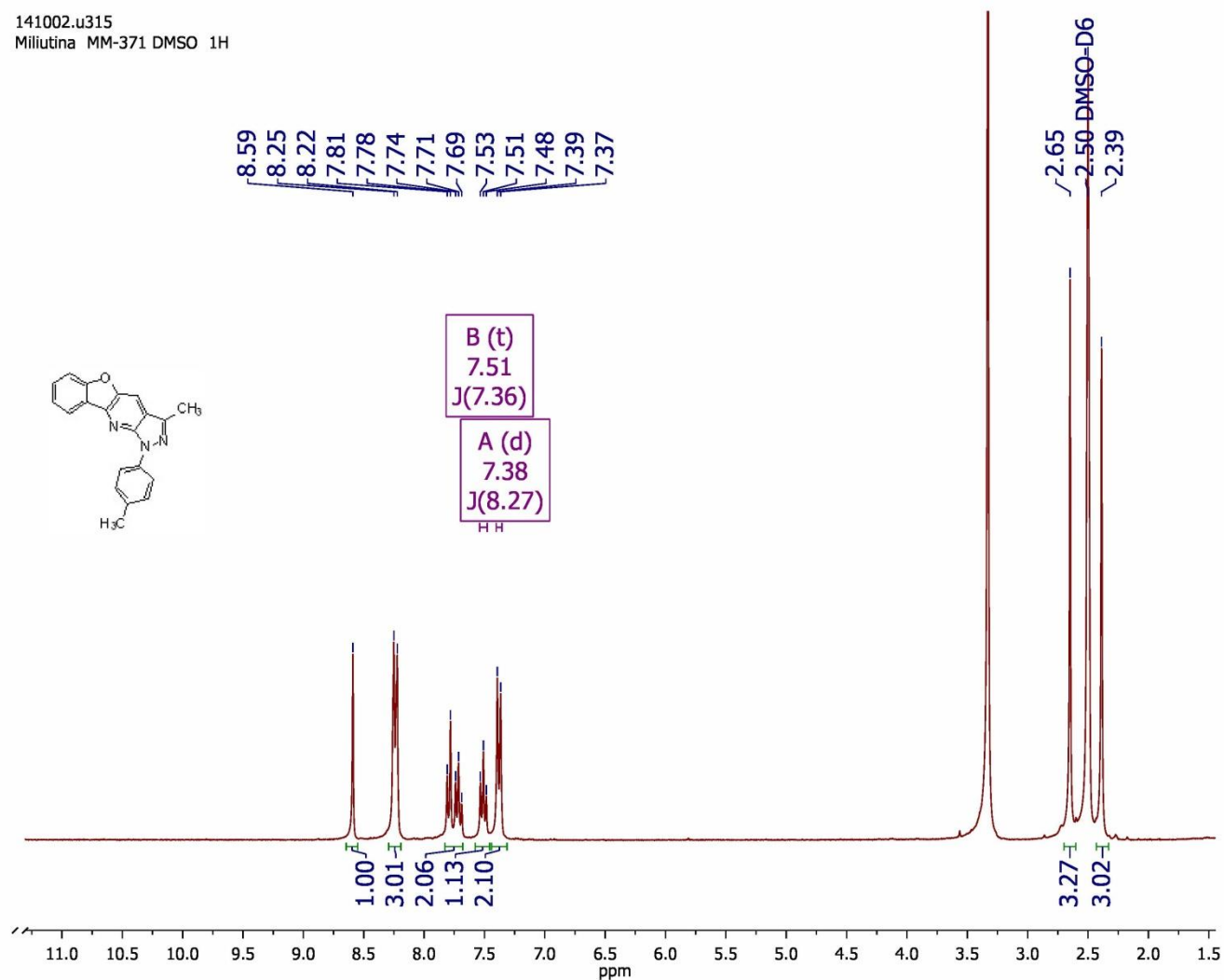
Millutina MM-291-1 13C DMSO



|                        |                                                                                    |
|------------------------|------------------------------------------------------------------------------------|
| Data File Name         | C:/Users/ë/Desktop/Спектры/ B/ 3-Cl-chromone/ MM-291/ 130912.202/ 10/ pdata/ 1/ 1r |
| Title                  | 130912.20                                                                          |
| Comment                | Millutina MM-291-1 13C DMSO                                                        |
| Origin                 | Bruker BioSpin GmbH                                                                |
| Owner                  | nmr                                                                                |
| Site                   |                                                                                    |
| Spectrometer           | spect                                                                              |
| Author                 |                                                                                    |
| Solvent                | DMSO                                                                               |
| Temperature            | 298.2                                                                              |
| Pulse Sequence         | zgpg30                                                                             |
| Number of Scans        | 1024                                                                               |
| Receiver Gain          | 2050                                                                               |
| Relaxation Delay       | 2.0000                                                                             |
| Pulse Width            | 10.2000                                                                            |
| Acquisition Time       | 2.1846                                                                             |
| Acquisition Date       | 2013-09-12T19:27:00                                                                |
| Modification Date      | 2013-09-12T18:28:36                                                                |
| Spectrometer Frequency | 62.90                                                                              |
| Spectral Width         | 15000.0                                                                            |
| Lowest Frequency       | -1238.3                                                                            |
| Nucleus                | 13C                                                                                |
| Acquired Size          | 32768                                                                              |
| Spectral Size          | 32768                                                                              |

### 3-Methyl-1-*p*-tolyl-1*H*-benzofuro[3,2-*b*]pyrazolo[4,3-*e*]pyridine (4b).

141002.u315  
Miliutina MM-371 DMSO 1H



Data File Name C:/Users/è/Desktop/Спектры/ C/3-Cl-chromone/MM-371/141002.u315/10/ fid

Title 141002.u315

Comment Miliutina MM-371 DMSO 1H

Origin Bruker BioSpin GmbH

Owner nmrsu

Site

Spectrometer spect

Author

Solvent DMSO

Temperature 298.2

Pulse zg30

Sequence

Number of Scans 16

Receiver Gain 144

Relaxation Delay 1.0000

Pulse Width 10.0000

Acquisition Time 5.2954

Acquisition Date 2014-10-02T1 3:23:00

Modification Date 2014-10-02T1 2:23:14

Spectrometer Frequency 300.13

Spectral Width 6188.1

Lowest Frequency -1242.1

Nucleus 1H

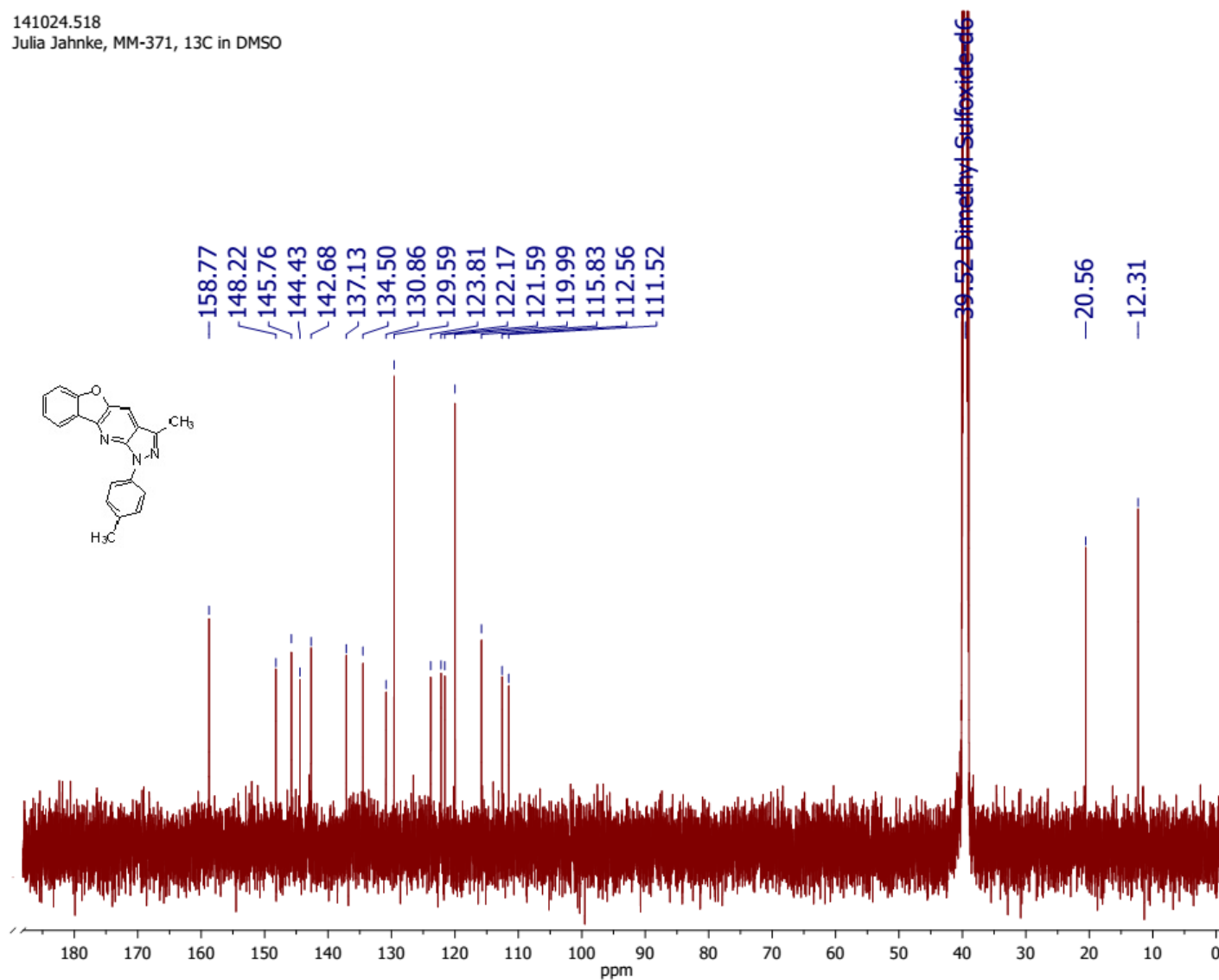
Acquired Size 32768

Spectral Size 65536

### 3-Methyl-1-*p*-tolyl-1*H*-benzofuro[3,2-*b*]pyrazolo[4,3-*e*]pyridine (4b).

141024.518

Julia Jahnke, MM-371, 13C in DMSO

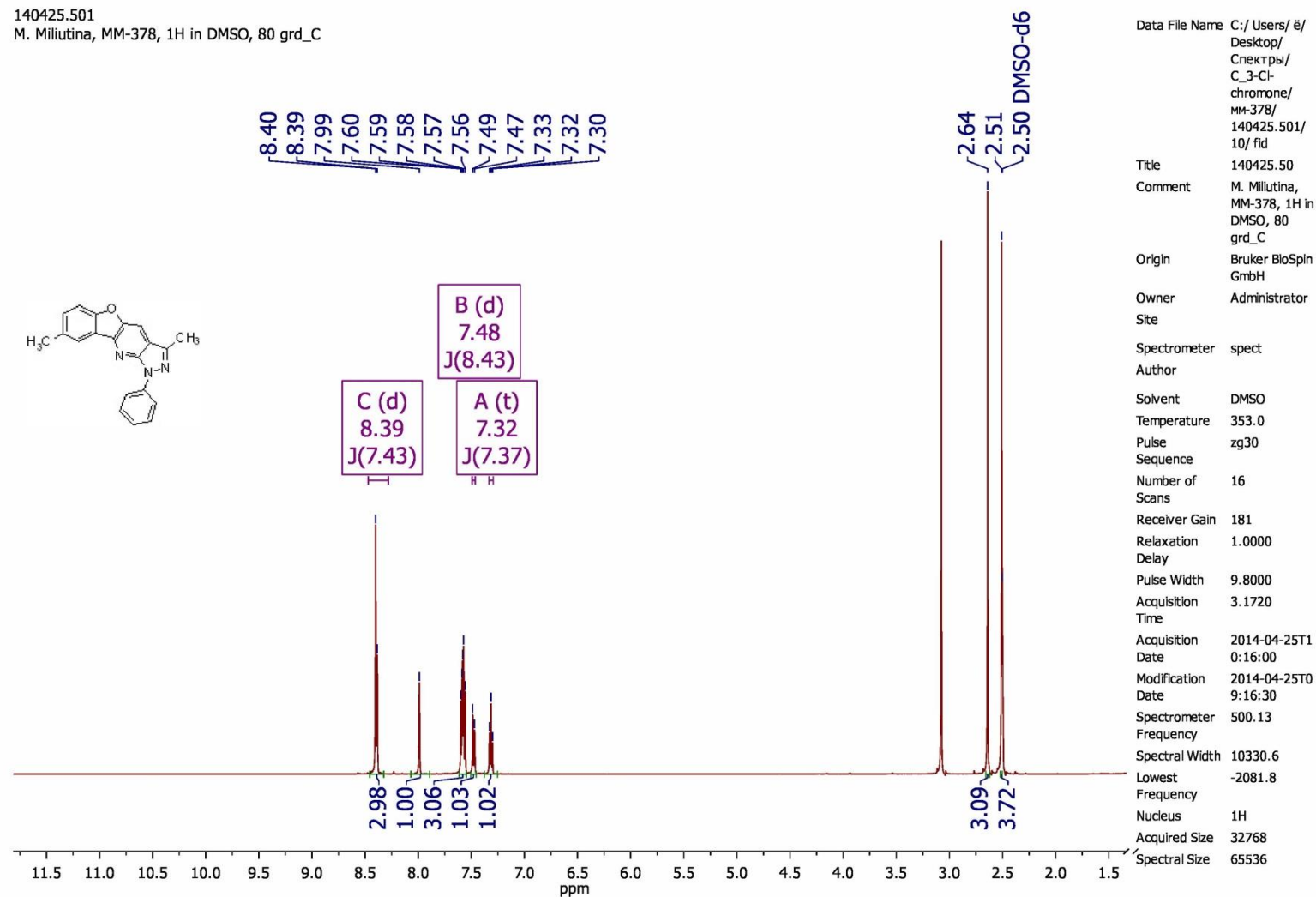


|                        |                                                     |
|------------------------|-----------------------------------------------------|
| Data File Name         | C:/Users/ë/Desktop/Спектры/1a/ 1/141024.518/14/ fid |
| Title                  | 141024.52                                           |
| Comment                | Julia Jahnke, MM-371, 13C in DMSO                   |
| Origin                 | Bruker BioSpin GmbH                                 |
| Owner                  | Administrator                                       |
| Site                   |                                                     |
| Spectrometer           | spect                                               |
| Author                 |                                                     |
| Solvent                | DMSO                                                |
| Temperature            | 300.0                                               |
| Pulse Sequence         | zgpg30                                              |
| Number of Scans        | 1024                                                |
| Receiver Gain          | 16384                                               |
| Relaxation Delay       | 2.0000                                              |
| Pulse Width            | 9.0000                                              |
| Acquisition Time       | 1.0912                                              |
| Acquisition Date       | 2014-10-24T 14:33:00                                |
| Modification Date      | 2014-10-24T 13:33:16                                |
| Spectrometer Frequency | 125.76                                              |
| Spectral Width         | 30030.0                                             |
| Lowest Frequency       | -2498.9                                             |
| Nucleus                | 13C                                                 |
| Acquired Size          | 32768                                               |
| Spectral Size          | 65536                                               |

### 3,8-Dimethyl-1-phenyl-1H-benzofuro[3,2-b]pyrazolo[4,3-e]pyridine (4c).

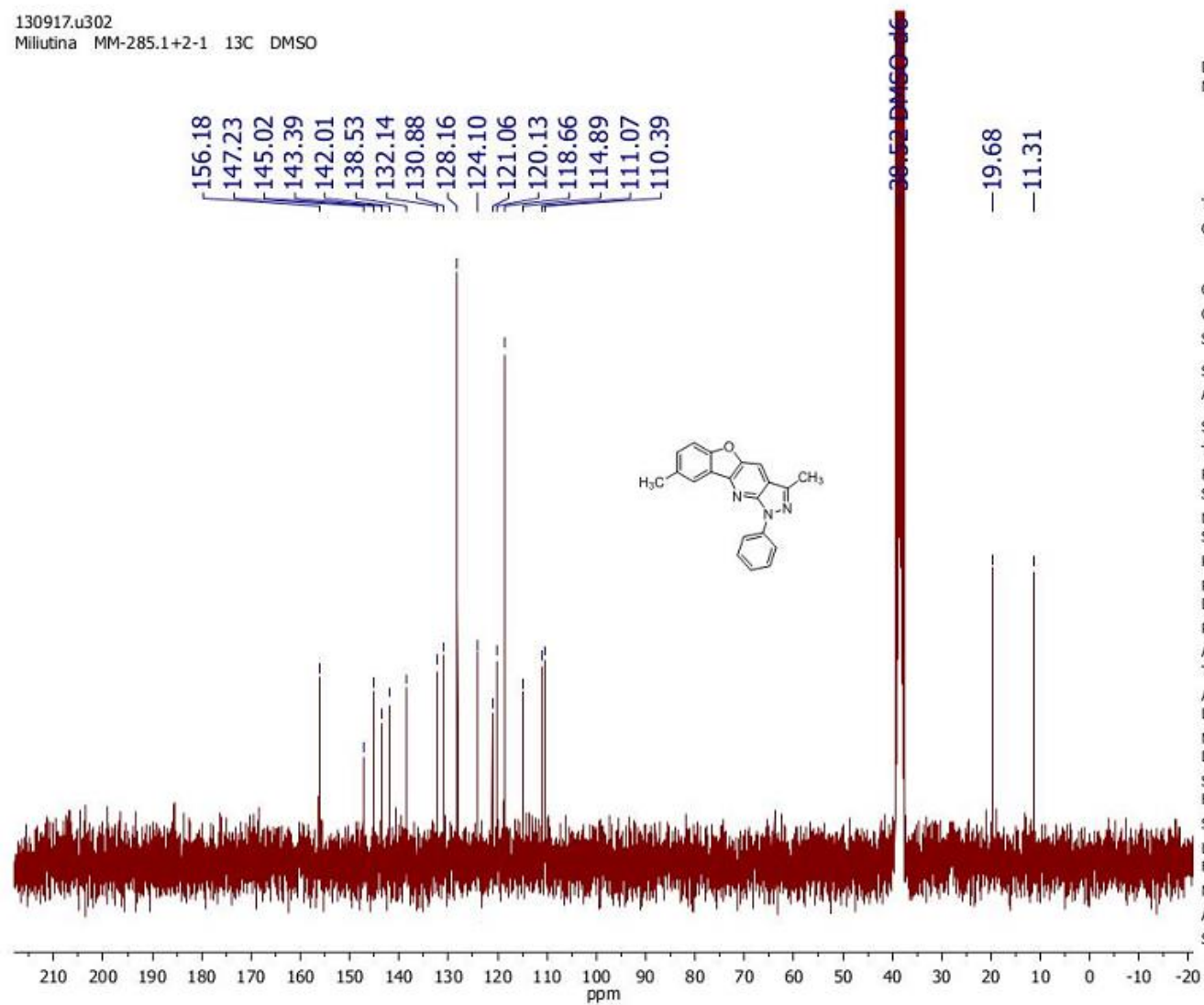
140425.501

M. Millutina, MM-378, 1H in DMSO, 80 grd\_C



### 3,8-Dimethyl-1-phenyl-1*H*-benzofuro[3,2-*b*]pyrazolo[4,3-*e*]pyridine (4c).

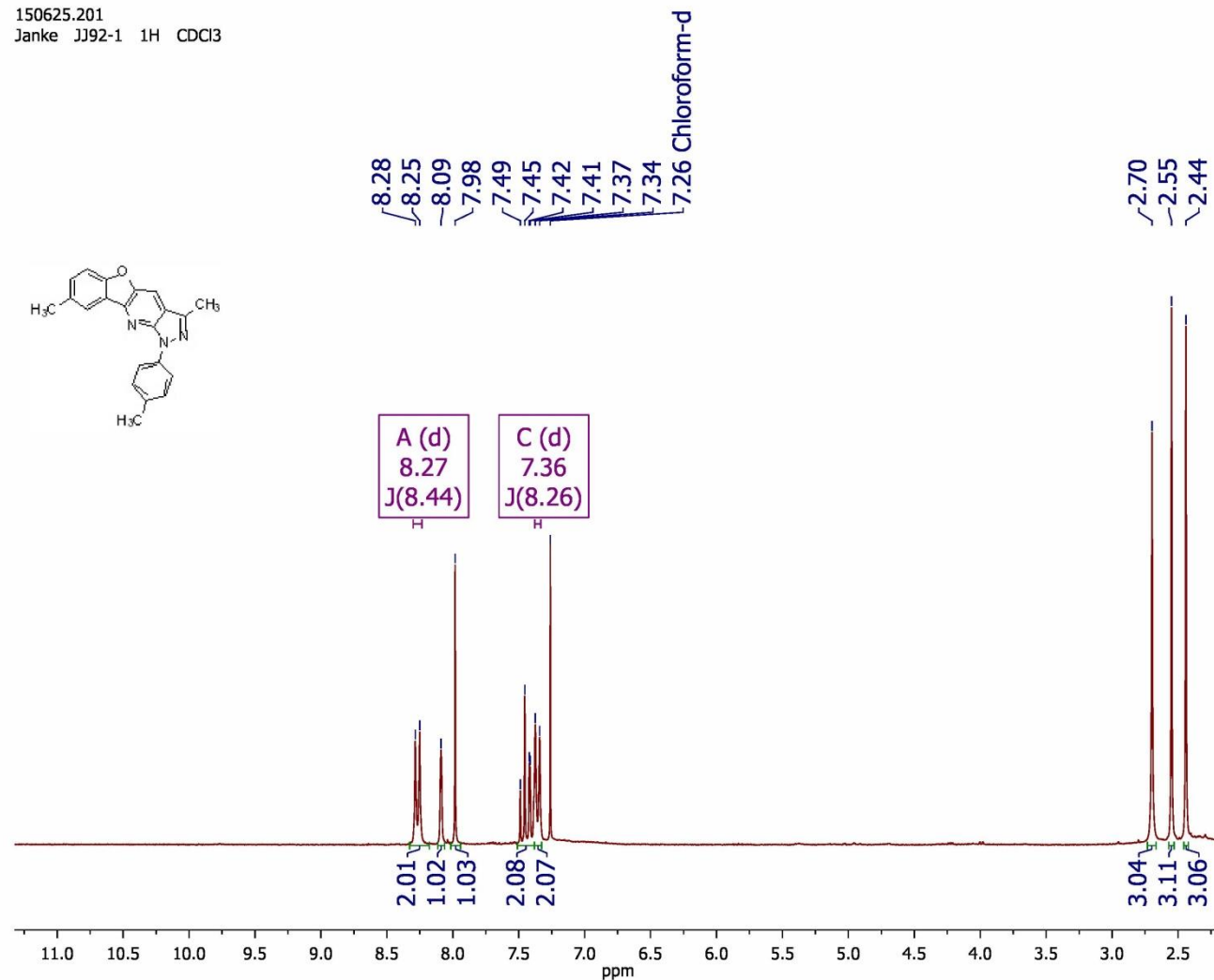
130917.u302  
Miliutina MM-285.1+2-1 13C DMSO



|                        |                                                                                              |
|------------------------|----------------------------------------------------------------------------------------------|
| Data File Name         | C:/Users/6/Desktop/Спектры/В/3-Cl-chromone/ММ-285.1+2/285.1+2-1/130917.u302/ 12/pdata/ 1/ 1r |
| Title                  | 130917.u302                                                                                  |
| Comment                | Miliutina MM-285.1+2-1 13C DMSO                                                              |
| Origin                 | Bruker BioSpin GmbH                                                                          |
| Owner                  | nmrsu                                                                                        |
| Site                   |                                                                                              |
| Spectrometer           | spect                                                                                        |
| Author                 |                                                                                              |
| Solvent                | DMSO                                                                                         |
| Temperature            | 298.4                                                                                        |
| Pulse                  | zgpg30                                                                                       |
| Sequence               |                                                                                              |
| Number of Scans        | 1024                                                                                         |
| Receiver Gain          | 2050                                                                                         |
| Relaxation Delay       | 2.0000                                                                                       |
| Pulse Width            | 10.0000                                                                                      |
| Acquisition Time       | 1.8176                                                                                       |
| Acquisition Date       | 2013-09-17T18:02:00                                                                          |
| Modification Date      | 2013-09-17T17:02:48                                                                          |
| Spectrometer Frequency | 75.47                                                                                        |
| Spectral Width         | 18028.8                                                                                      |
| Lowest Frequency       | -1582.2                                                                                      |
| Nucleus                | 13C                                                                                          |
| Acquired Size          | 32768                                                                                        |
| Spectral Size          | 32768                                                                                        |

# 3,8-Dimethyl-1-*p*-tolyl-1*H*-benzofuro[3,2-*b*]pyrazolo[4,3-*e*]pyridine (4d).

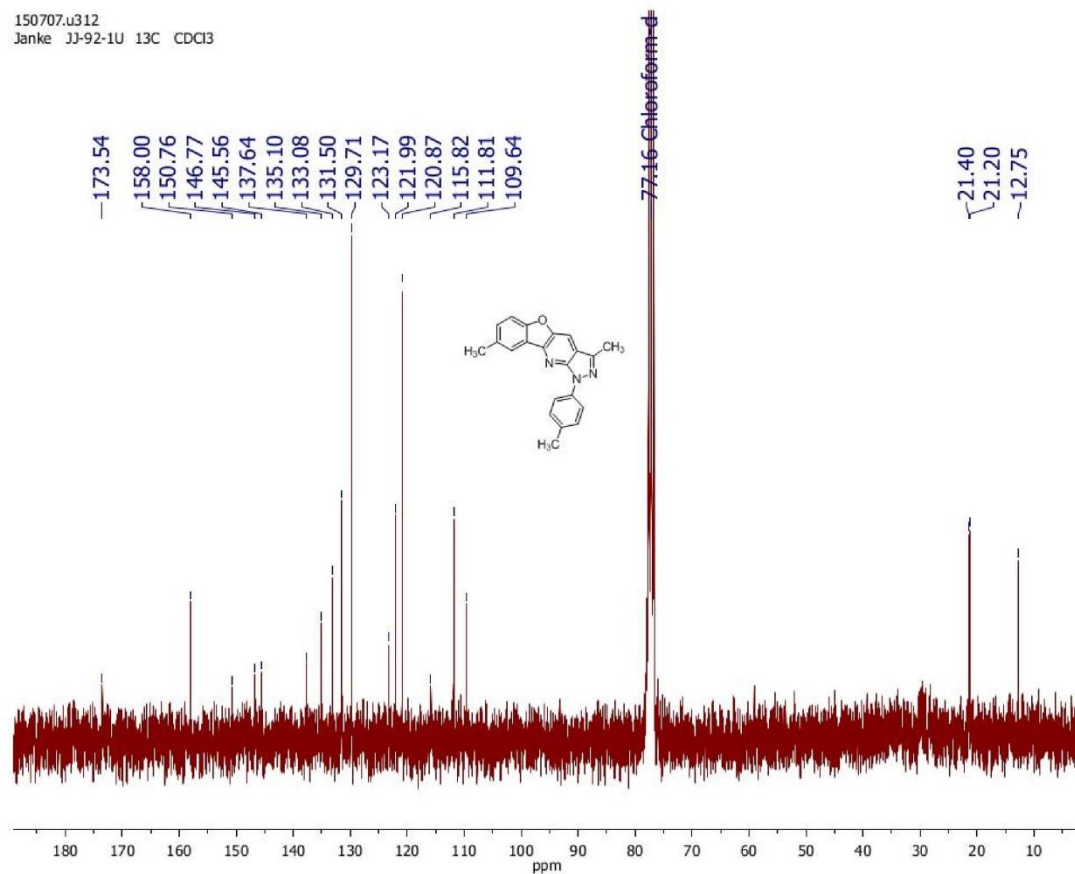
150625.201  
Janke JJ92-1 1H CDCl3



|                        |                                                                               |
|------------------------|-------------------------------------------------------------------------------|
| Data File Name         | C:/Users/è/Desktop/Спектры/ C/3-Cl-chromone/JJ-92/ JJ-92/ 150625.201/ 10/ fid |
| Title                  | 150625.20                                                                     |
| Comment                | Janke JJ92-1 1H CDCl3                                                         |
| Origin                 | Bruker BioSpin GmbH                                                           |
| Owner Site             | nmr                                                                           |
| Spectrometer Author    | spect                                                                         |
| Solvent                | CDCl3                                                                         |
| Temperature            | 298.1                                                                         |
| Pulse                  | zg30                                                                          |
| Sequence               |                                                                               |
| Number of Scans        | 16                                                                            |
| Receiver Gain          | 645                                                                           |
| Relaxation Delay       | 1.0000                                                                        |
| Pulse Width            | 11.4000                                                                       |
| Acquisition Time       | 6.3439                                                                        |
| Acquisition Date       | 2015-06-25T09:59:00                                                           |
| Modification Date      | 2015-06-25T09:00:20                                                           |
| Spectrometer Frequency | 250.13                                                                        |
| Spectral Width         | 5165.3                                                                        |
| Lowest Frequency       | -1038.6                                                                       |
| Nucleus                | 1H                                                                            |
| Acquired Size          | 32768                                                                         |
| Spectral Size          | 65536                                                                         |

# 3,8-Dimethyl-1-*p*-tolyl-1*H*-benzofuro[3,2-*b*]pyrazolo[4,3-*e*]pyridine (4d).

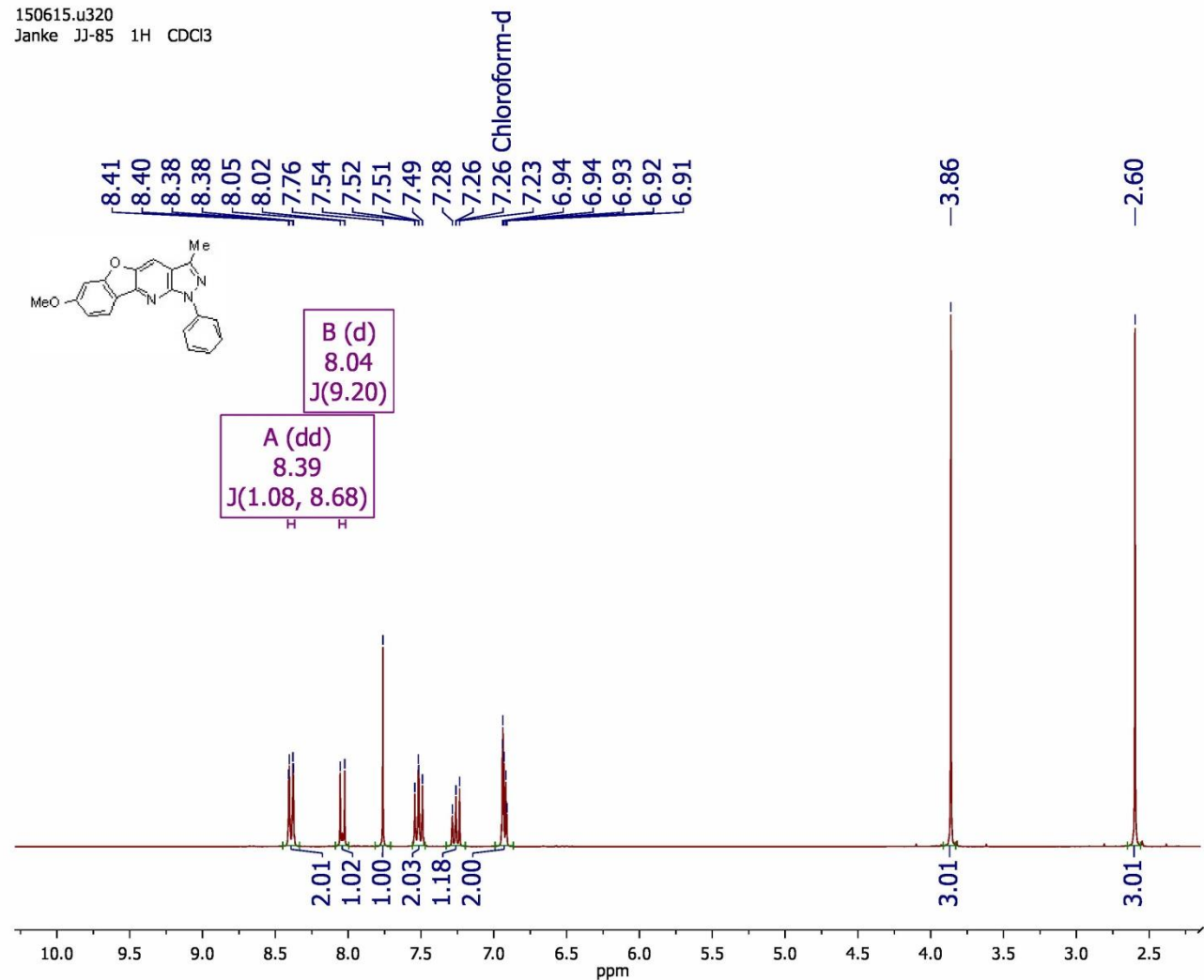
150707.u312  
Janke JJ-92-1U 13C CDCl3



|                |                |
|----------------|----------------|
| Data File      | C:/Users/E/    |
| Name           | Desktop/       |
|                | Chetru/C/      |
|                | 3-Cl-          |
|                | chromone/      |
|                | JJ-92/         |
|                | JJ-92-1/       |
|                | 150707.u312/   |
|                | 150707.u312/   |
|                | 11/fid         |
| Title          | 150707.u312    |
| Comment        | Janke          |
|                | JJ-92-1U 13C   |
|                | CDCl3          |
| Origin         | Bruker BioSpin |
| Owner          | GmbH           |
| Site           | nmrsu          |
| Spectrometer   | spect          |
| Author         |                |
| Solvent        | CDCl3          |
| Temperature    | 300.0          |
| Pulse          | zgpg30         |
| Sequence       |                |
| Number of      | 1024           |
| Scans          |                |
| Receiver Gain  | 2050           |
| Relaxation     | 2.0000         |
| Delay          |                |
| Pulse Width    | 10.0000        |
| Acquisition    | 1.8176         |
| Time           |                |
| Acquisition    | 2015-07-08T0   |
| Date           | 6:06:00        |
| Modification   | 2015-07-08T0   |
| Date           | 5:06:06        |
| Spectrometer   | 75.47          |
| Frequency      |                |
| Spectral Width | 18028.8        |
| Lowest         | -1456.7        |
| Frequency      |                |
| Nucleus        | 13C            |
| Acquired Size  | 32768          |
| Spectral Size  | 65536          |

# 7-Methoxy-3-methyl-1-phenyl-1H-benzofuro[3,2-b]pyrazolo[4,3-e]pyridine (4e).

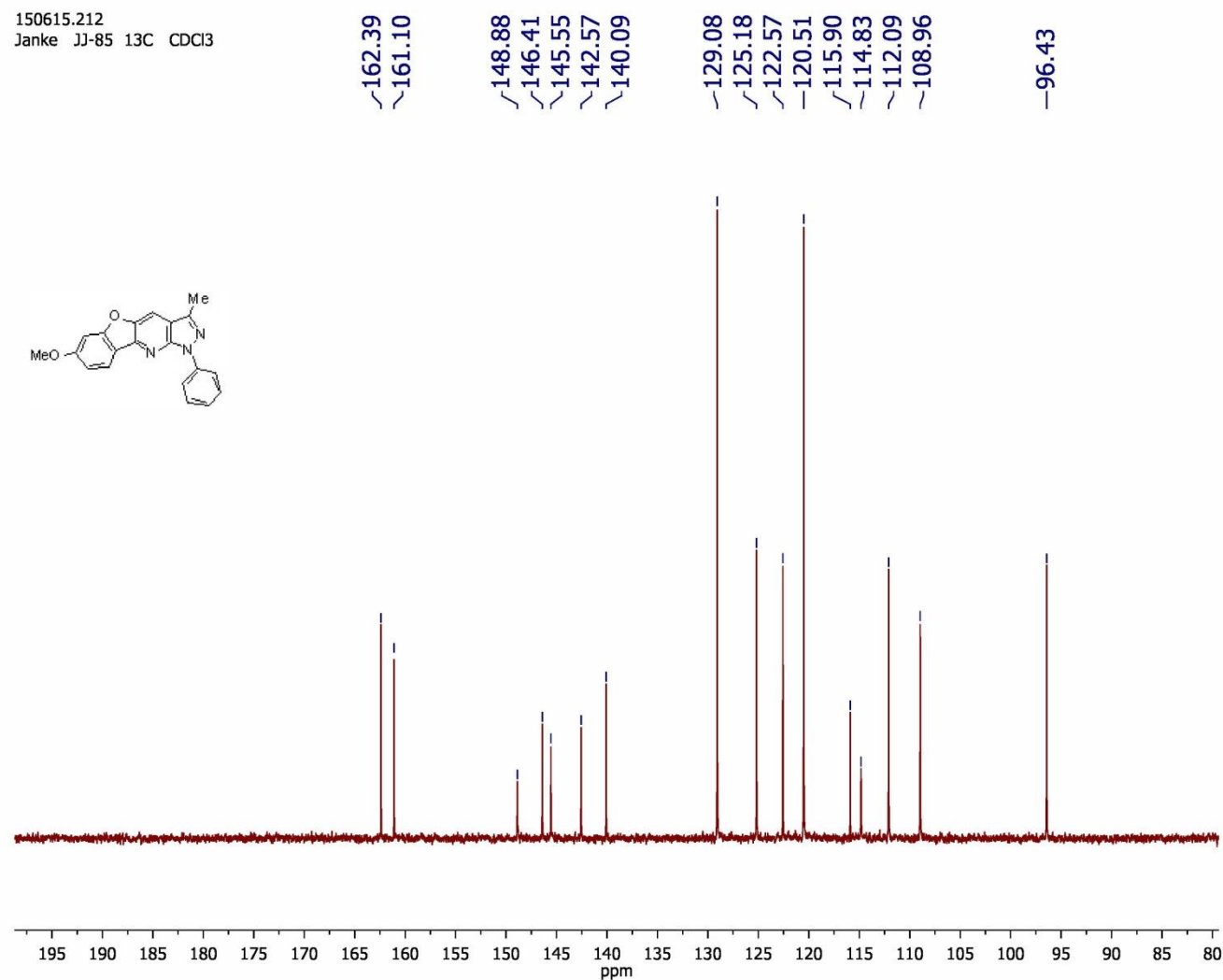
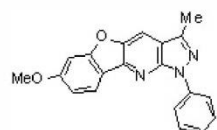
150615.u320  
Janke JJ-85 1H CDCl3



|                        |                                                                             |
|------------------------|-----------------------------------------------------------------------------|
| Data File Name         | C:/Users/ě/Desktop/Спектры/ C/3-Cl-chromone/JJ-85/JJ-85/150615.u320/10/ fid |
| Title                  | 150615.u320                                                                 |
| Comment                | Janke JJ-85 1H CDCl3                                                        |
| Origin                 | Bruker BioSpin GmbH                                                         |
| Owner                  | nrrsu                                                                       |
| Site                   |                                                                             |
| Spectrometer           | spect                                                                       |
| Author                 |                                                                             |
| Solvent                | CDCl3                                                                       |
| Temperature            | 298.2                                                                       |
| Pulse                  | zg30                                                                        |
| Sequence               |                                                                             |
| Number of Scans        | 16                                                                          |
| Receiver Gain          | 51                                                                          |
| Relaxation Delay       | 1.0000                                                                      |
| Pulse Width            | 10.0000                                                                     |
| Acquisition Time       | 5.2954                                                                      |
| Acquisition Date       | 2015-06-15T12:37:00                                                         |
| Modification Date      | 2015-06-15T11:37:04                                                         |
| Spectrometer Frequency | 300.13                                                                      |
| Spectral Width         | 6188.1                                                                      |
| Lowest Frequency       | -1404.6                                                                     |
| Nucleus                | 1H                                                                          |
| Acquired Size          | 32768                                                                       |
| Spectral Size          | 65536                                                                       |

# 7-Methoxy-3-methyl-1-phenyl-1H-benzofuro[3,2-b]pyrazolo[4,3-e]pyridine (4e).

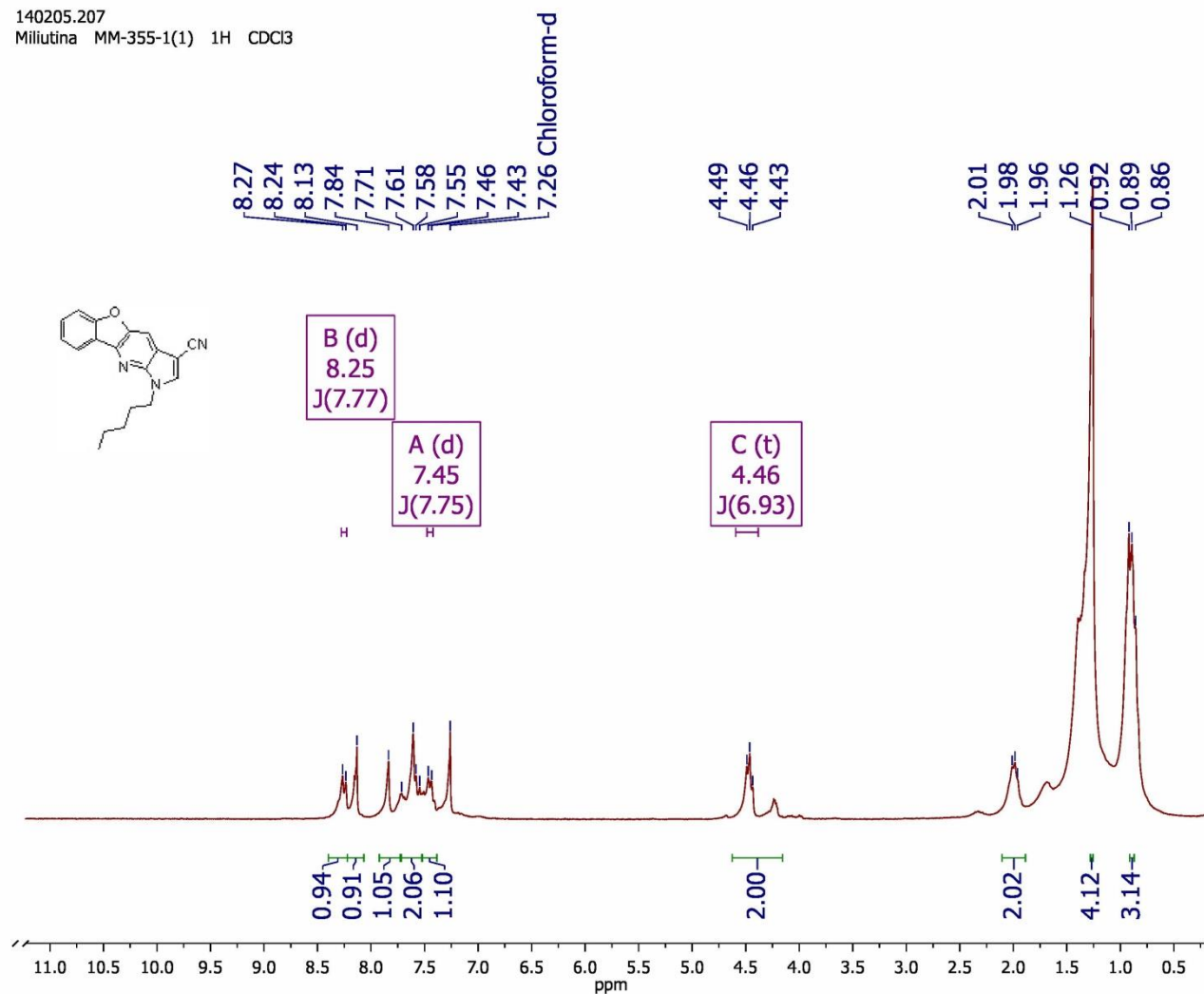
150615.212  
Janke JJ-85 13C CDCl3



Data File Name: C:/Users/8/Desktop/Спектры/ C/3-Cl-chromone/JJ-85/ JJ-85/150615.212/10/ fid  
Title: 150615.21  
Comment: Janke JJ-85 13C CDCl3  
Origin: Bruker BioSpin GmbH  
Owner: nmr  
Site:  
Spectrometer: spect  
Author:  
Solvent: CDCl3  
Temperature: 298.1  
Pulse: zgpg30  
Sequence:  
Number of Scans: 1024  
Receiver Gain: 2050  
Relaxation: 2.0000  
Delay:  
Pulse Width: 10.2000  
Acquisition Time: 2.1846  
Acquisition Date: 2015-06-16T 01:39:00  
Modification Date: 2015-06-16T 00:40:08  
Spectrometer Frequency: 62.90  
Spectral Width: 15000.0  
Lowest Frequency: -1203.4  
Nucleus: 13C  
Acquired Size: 32768  
Spectral Size: 65536

# 1-Pentyl-1*H*-benzofuro[3,2-*b*]pyrrolo[3,2-*e*]pyridine-3-carbonitrile (4f).

140205.207  
Miliutina MM-355-1(1) 1H CDCl3



Data File Name C:/Users/E/  
Desktop/  
Спектры/ C/ 3-  
Cl-chromone/  
MM-355/  
355-1(1)/  
140205.207/  
140205.207/  
10/ fid

Title 140205.21

Comment Miliutina  
MM-355-1(1) 1H  
CDCl3

Origin Bruker BioSpin  
GmbH

Owner nmr

Site

Spectrometer spect

Author

Solvent CDCl3

Temperature 298.2

Pulse Sequence zg30

Number of Scans 32

Receiver Gain 322

Relaxation Delay 1.0000

Pulse Width 10.0000

Acquisition Time 6.3439

Acquisition Date 2014-02-05T19:  
57:00

Modification 2014-02-05T19:  
58:26

Date

Spectrometer 250.13

Frequency

Spectral Width 5165.3

Lowest -1035.0

Frequency

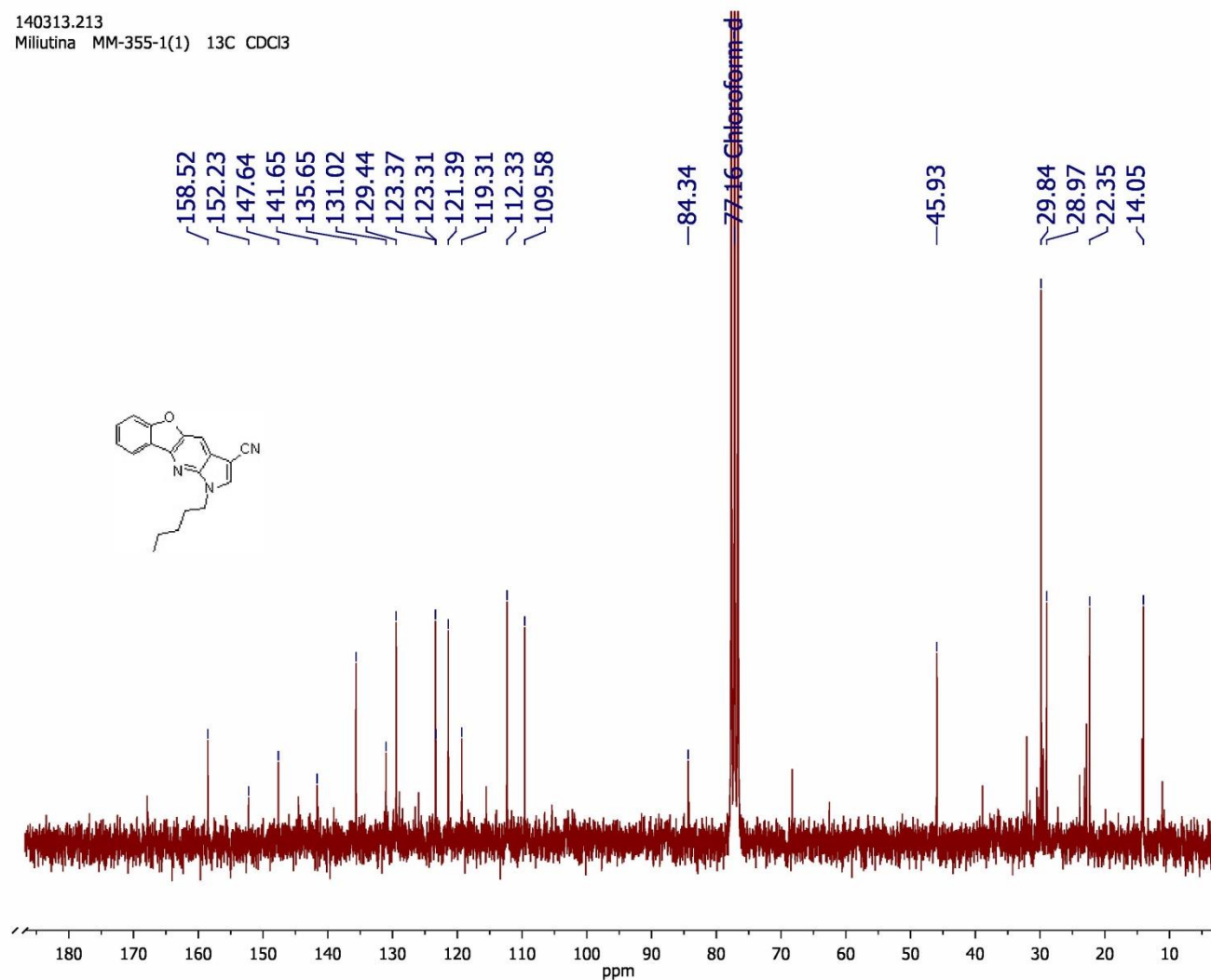
Nucleus 1H

Acquired Size 32768

Spectral Size 65536

# 1-Pentyl-1*H*-benzofuro[3,2-*b*]pyrrolo[3,2-*e*]pyridine-3-carbonitrile (4f).

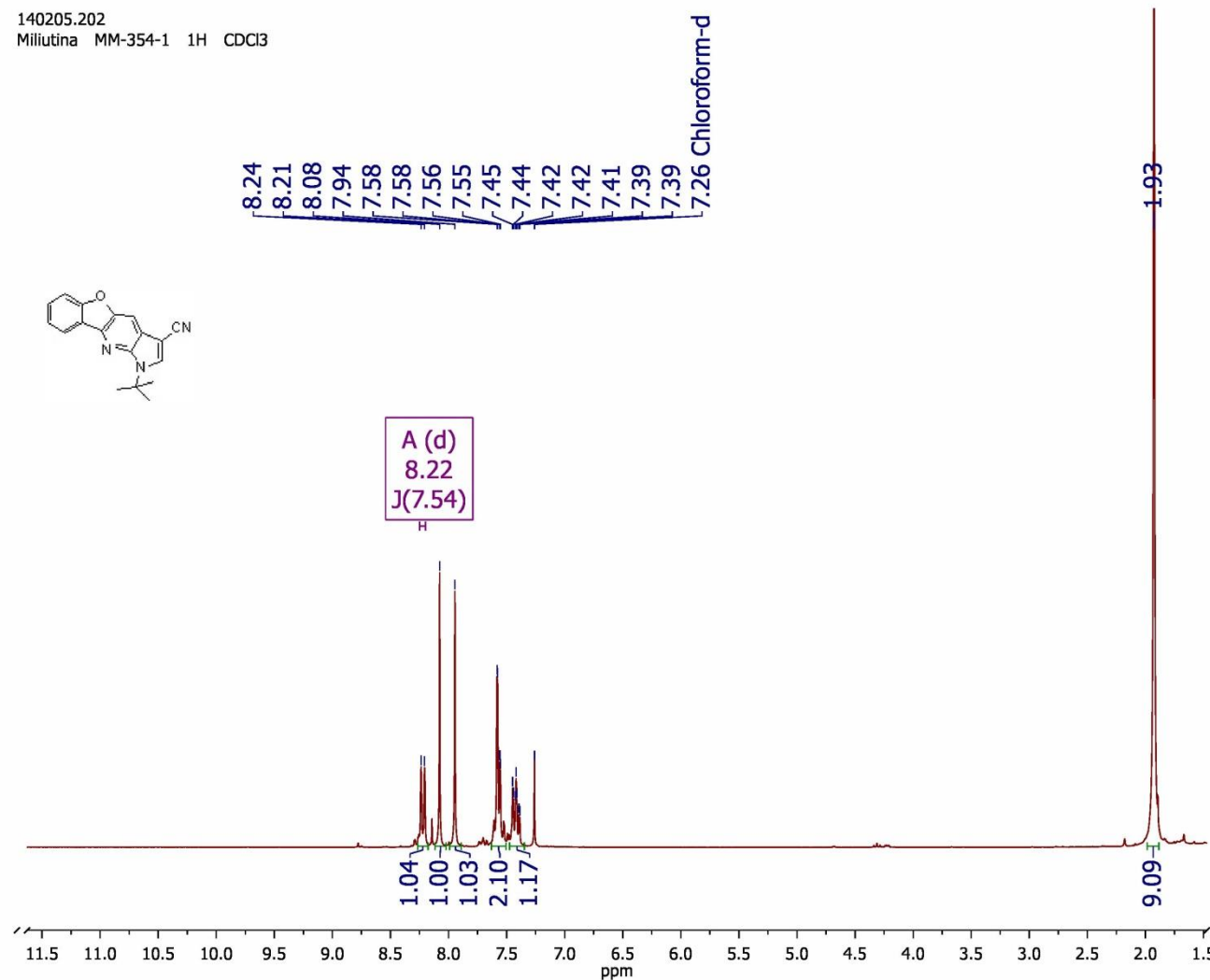
140313.213  
Miliutina MM-355-1(1) 13C CDCl<sub>3</sub>



|                        |                                                                                                |
|------------------------|------------------------------------------------------------------------------------------------|
| Data File Name         | C:/Users/ë/Desktop/Спектры/ C/3-Cl-chromone/ MM-355/ 355-1(1)/ 140313.213/ 140313.213/ 12/ fid |
| Title                  | 140313.21                                                                                      |
| Comment                | Miliutina MM-355-1(1) 13C CDCl <sub>3</sub>                                                    |
| Origin                 | Bruker BioSpin GmbH                                                                            |
| Owner                  | nmr                                                                                            |
| Site                   |                                                                                                |
| Spectrometer           | spect                                                                                          |
| Author                 |                                                                                                |
| Solvent                | CDCl <sub>3</sub>                                                                              |
| Temperature            | 298.0                                                                                          |
| Pulse                  | zgpg30                                                                                         |
| Sequence               |                                                                                                |
| Number of Scans        | 2048                                                                                           |
| Receiver Gain          | 2050                                                                                           |
| Relaxation Delay       | 2.0000                                                                                         |
| Pulse Width            | 10.0000                                                                                        |
| Acquisition Time       | 2.1846                                                                                         |
| Acquisition Date       | 2014-03-13T2 3:39:00                                                                           |
| Modification Date      | 2014-03-13T2 3:39:46                                                                           |
| Spectrometer Frequency | 62.90                                                                                          |
| Spectral Width         | 15000.0                                                                                        |
| Lowest Frequency       | -1274.1                                                                                        |
| Nucleus                | 13C                                                                                            |
| Acquired Size          | 32768                                                                                          |
| Spectral Size          | 65536                                                                                          |

**1-*tert*-Butyl-1*H*-benzofuro[3,2-*b*]pyrrolo[3,2-*e*]pyridine-3-carbonitrile (4g).**

140205.202  
Millutina MM-354-1 1H CDCl<sub>3</sub>



Data File Name C:/Users/ë/Desktop/Спектры/ C/3-Cl-chromone/ MM-354/ 354-1/ 140205.202/ 10/ fid

Title 140205.20

Comment Millutina MM-354-1 1H CDCl<sub>3</sub>

Origin Bruker BioSpin GmbH

Owner nmr

Site

Spectrometer spect

Author

Solvent CDCl<sub>3</sub>

Temperature 298.2

Pulse Sequence zg30

Number of Scans 16

Receiver Gain 322

Relaxation Delay 1.0000

Pulse Width 10.0000

Acquisition Time 6.3439

Acquisition Date 2014-02-05T1 1:08:00

Modification Date 2014-02-05T1 1:08:52

Spectrometer Frequency 250.13

Spectral Width 5165.3

Lowest Frequency -1038.3

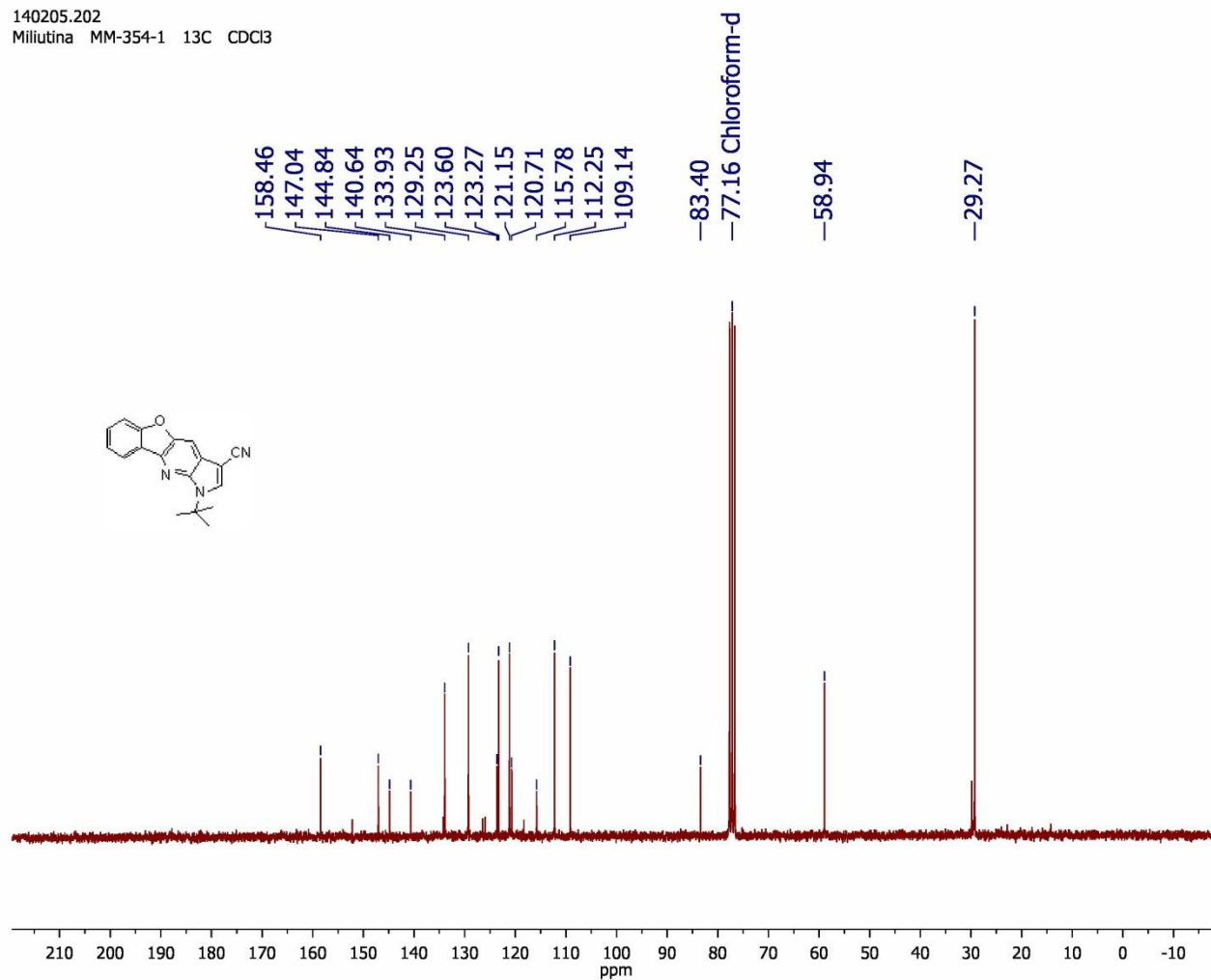
Nucleus 1H

Acquired Size 32768

Spectral Size 65536

**1-*tert*-Butyl-1*H*-benzofuro[3,2-*b*]pyrrolo[3,2-*e*]pyridine-3-carbonitrile (4g).**

140205.202  
Miliutina MM-354-1 13C CDCl<sub>3</sub>

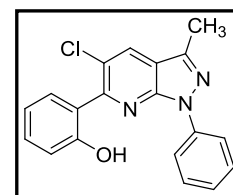
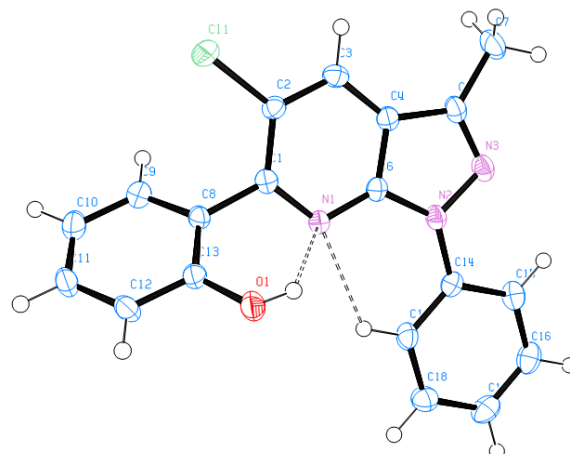


|                        |                                                                             |
|------------------------|-----------------------------------------------------------------------------|
| Data File Name         | C:/Users/è/Desktop/Спектры/ C/3-Cl-chromone/MM-354/354-1/140205.202/12/ fid |
| Title                  | 140205.20                                                                   |
| Comment                | Miliutina MM-354-1 13C CDCl <sub>3</sub>                                    |
| Origin                 | Bruker BioSpin GmbH                                                         |
| Owner                  | nmr                                                                         |
| Site                   |                                                                             |
| Spectrometer           | spect                                                                       |
| Author                 |                                                                             |
| Solvent                | CDCl <sub>3</sub>                                                           |
| Temperature            | 298.0                                                                       |
| Pulse Sequence         | zgpg30                                                                      |
| Number of Scans        | 1024                                                                        |
| Receiver Gain          | 2050                                                                        |
| Relaxation Delay       | 2.0000                                                                      |
| Pulse Width            | 10.0000                                                                     |
| Acquisition Time       | 2.1846                                                                      |
| Acquisition Date       | 2014-02-05T1 2:38:00                                                        |
| Modification Date      | 2014-02-05T1 2:39:18                                                        |
| Spectrometer Frequency | 62.90                                                                       |
| Spectral Width         | 15000.0                                                                     |
| Lowest Frequency       | -1206.1                                                                     |
| Nucleus                | 13C                                                                         |
| Acquired Size          | 32768                                                                       |
| Spectral Size          | 65536                                                                       |

## X-Ray structures of compounds 3a, 3m, 3o and 4c.

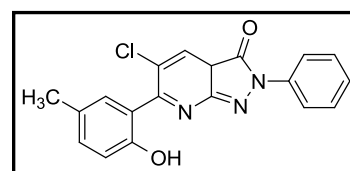
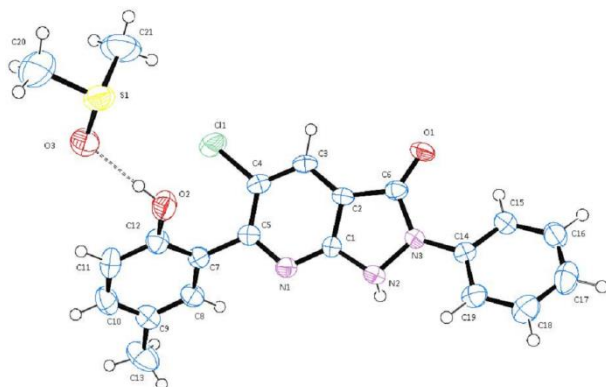
### X-Ray structure of compound 3a.

|                                        |                                                                                                                                                                          |
|----------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Identification Code                    | is_mm251                                                                                                                                                                 |
| Empirical formula                      | C <sub>19</sub> H <sub>14</sub> Cl N <sub>3</sub> O                                                                                                                      |
| Formula weight                         | 335.78                                                                                                                                                                   |
| Temperature                            | 173(2) K                                                                                                                                                                 |
| Wavelength                             | 0.71073 Å                                                                                                                                                                |
| Crystal system                         | monoclinic                                                                                                                                                               |
| Space group (H.-M.)                    | <i>P</i> 2 <sub>1</sub> / <i>c</i>                                                                                                                                       |
| Space group (Hall)                     | - <i>P</i> 2ybc                                                                                                                                                          |
| Unit cell dimensions                   | $a = 12.6542(8) \text{ Å}$<br>$b = 6.7364(4) \text{ Å}$<br>$c = 18.7735(12) \text{ Å}$<br>$\alpha = 90.00^\circ$<br>$\beta = 103.364(3)^\circ$<br>$\gamma = 90.00^\circ$ |
| Volume                                 | 1556.99(17) Å <sup>3</sup>                                                                                                                                               |
| Z                                      | 4                                                                                                                                                                        |
| Calculated density                     | 1.432 Mg/m <sup>3</sup>                                                                                                                                                  |
| Absorption coefficient                 | 0.256 mm <sup>-1</sup>                                                                                                                                                   |
| F(000)                                 | 696                                                                                                                                                                      |
| Crystal size                           | 0.99 x 0.04 x 0.03 mm <sup>3</sup>                                                                                                                                       |
| $\Theta$ range for data collection     | 3.07 to 27.50°                                                                                                                                                           |
| Index ranges                           | -16 ≤ <i>h</i> ≤ 16, -8 ≤ <i>k</i> ≤ 5, -24 ≤ <i>l</i> ≤ 24                                                                                                              |
| Reflections collected                  | 16946                                                                                                                                                                    |
| Independent reflections                | 3568 [R(int) = 0.0960]                                                                                                                                                   |
| Completeness to $\Theta = 28.00^\circ$ | 99.7%                                                                                                                                                                    |
| Absorption correction                  | Multi-scan                                                                                                                                                               |
| Max. and min. transmission             | 0.9924 and 0.7857                                                                                                                                                        |
| Refinement method                      | Full-matrix least-squares on F <sup>2</sup>                                                                                                                              |
| Data / restraints / parameters         | 2134 / 0 / 222                                                                                                                                                           |
| Goodness-of-fit on F <sup>2</sup>      | 1.033                                                                                                                                                                    |
| Final R indices [I > 2σ(I)]            | R1 = 0.0623, wR2 = 0.1084                                                                                                                                                |
| R indices (all data)                   | R1 = 0.1236, wR2 = 0.1338                                                                                                                                                |
| Largest diff. peak and hole            | 0.320 and -0.291 e.Å <sup>-3</sup>                                                                                                                                       |



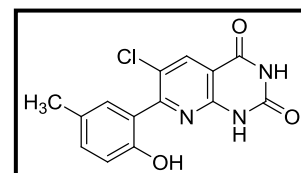
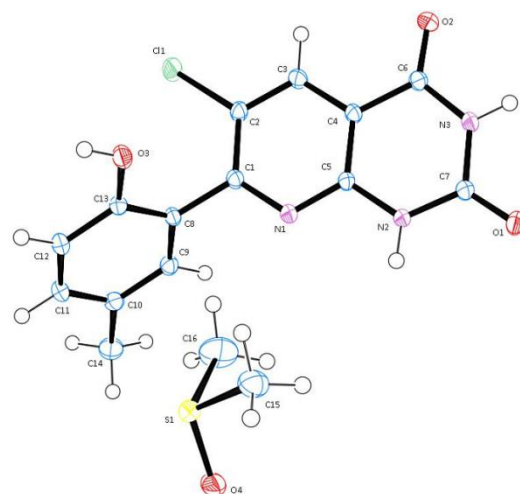
### X-Ray structure of compound 3m.

|                                        |                                                                                                                                        |
|----------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| Identification Code                    | is_mm353                                                                                                                               |
| Empirical formula                      | C <sub>21</sub> H <sub>20</sub> Cl N <sub>3</sub> O <sub>3</sub> S                                                                     |
| Formula weight                         | 429.91                                                                                                                                 |
| Temperature                            | 173(2) K                                                                                                                               |
| Wavelength                             | 0.71073 Å                                                                                                                              |
| Crystal system                         | monoclinic                                                                                                                             |
| Space group (H.-M.)                    | <i>P</i> 2 <sub>1</sub> /c                                                                                                             |
| Space group (Hall)                     | -P 2ybc                                                                                                                                |
| Unit cell dimensions                   | $a = 20.255(10)$ Å<br>$b = 7.228(4)$ Å<br>$c = 14.842(8)$ Å<br>$\alpha = 90^\circ$<br>$\beta = 107.35(3)^\circ$<br>$\gamma = 90^\circ$ |
| Volume                                 | 2074(2) Å <sup>3</sup>                                                                                                                 |
| Z                                      | 4                                                                                                                                      |
| Calculated density                     | 1.377 Mg/m <sup>3</sup>                                                                                                                |
| Absorption coefficient                 | 0.313 mm <sup>-1</sup>                                                                                                                 |
| F(000)                                 | 896                                                                                                                                    |
| Crystal size                           | 0.480 x 0.150 x 0.010 mm <sup>3</sup>                                                                                                  |
| $\Theta$ range for data collection     | 2.876 to 22.362°                                                                                                                       |
| Index ranges                           | $-19 \leq h \leq 21$ , $-7 \leq k \leq 5$ , $-15 \leq l \leq 15$                                                                       |
| Reflections collected                  | 14125                                                                                                                                  |
| Independent reflections                | 2637 [R(int) = 0.0854]                                                                                                                 |
| Completeness to $\Theta = 28.00^\circ$ | 98,9%                                                                                                                                  |
| Absorption correction                  | Multi-scan                                                                                                                             |
| Max. and min. transmission             | 0.7448 and 0.6520                                                                                                                      |
| Refinement method                      | Full-matrix least-squares on F <sup>2</sup>                                                                                            |
| Data / restraints / parameters         | 1575 / 6 / 282                                                                                                                         |
| Goodness-of-fit on F <sup>2</sup>      | 1.030                                                                                                                                  |
| Final R indices [I>2sigma(I)]          | R1 = 0.0491, wR2 = 0.0970                                                                                                              |
| R indices (all data)                   | R1 = 0.1086, wR2 = 0.1205                                                                                                              |
| Largest diff. peak and hole            | 0.217 and -0.326 e.Å <sup>-3</sup>                                                                                                     |



### X-Ray structure of compound 3o.

|                                   |                                                                                                                                                                                     |
|-----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Identification Code               | is_mm258                                                                                                                                                                            |
| Empirical formula                 | C <sub>16</sub> H <sub>16</sub> Cl N <sub>3</sub> O <sub>4</sub> S                                                                                                                  |
| Formula weight                    | 381.83                                                                                                                                                                              |
| Temperature                       | 173(2) K                                                                                                                                                                            |
| Wavelength                        | 0.71073 Å                                                                                                                                                                           |
| Crystal system                    | triclinic                                                                                                                                                                           |
| Space group (H.-M.)               | $P\bar{1}$                                                                                                                                                                          |
| Space group (Hall)                | -P 1                                                                                                                                                                                |
| Unit cell dimensions              | $a = 7.2883(2) \text{ Å}$<br>$b = 7.8141(2) \text{ Å}$<br>$c = 15.5616(3) \text{ Å}$<br>$\alpha = 78.2630(10)^\circ$<br>$\beta = 86.7750(10)^\circ$<br>$\gamma = 76.9220(10)^\circ$ |
| Volume                            | 845.17(4) Å <sup>3</sup>                                                                                                                                                            |
| Z                                 | 2                                                                                                                                                                                   |
| Calculated density                | 1.500 Mg/m <sup>3</sup>                                                                                                                                                             |
| Absorption coefficient            | 0.377 mm <sup>-1</sup>                                                                                                                                                              |
| F(000)                            | 396                                                                                                                                                                                 |
| Crystal size                      | 0.290 x 0.230 x 0.060 mm <sup>3</sup>                                                                                                                                               |
| Θ range for data collection       | 2.674 to 32.500°                                                                                                                                                                    |
| Index ranges                      | -10 ≤ h ≤ 11, -11 ≤ k ≤ 11, -23 ≤ l ≤ 23                                                                                                                                            |
| Reflections collected             | 27106                                                                                                                                                                               |
| Independent reflections           | 6050 [R(int) = 0.0233]                                                                                                                                                              |
| Completeness to Θ = 28.00°        | 99,0%                                                                                                                                                                               |
| Absorption correction             | Multi-scan                                                                                                                                                                          |
| Max. and min. transmission        | 0.7464 and 0.6974                                                                                                                                                                   |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                                                                                                                                         |
| Data / restraints / parameters    | 4834 / 0 / 241                                                                                                                                                                      |
| Goodness-of-fit on F <sup>2</sup> | 1.039                                                                                                                                                                               |
| Final R indices [I>2σ(I)]         | R1 = 0.0390, wR2 = 0.0941                                                                                                                                                           |
| R indices (all data)              | R1 = 0.0550, wR2 = 0.1038                                                                                                                                                           |
| Largest diff. peak and hole       | 0.531 and -0.351 e.Å <sup>-3</sup>                                                                                                                                                  |



### X-Ray structure of compound 4c.

Identification Code ah\_mm378

Empirical formula C<sub>20</sub> H<sub>15</sub> N<sub>3</sub> O

Formula weight 313.35

Temperature 173(2) K

Wavelength 0.71073 Å

Crystal system monoclinic

Space group (H.-M.) *C* 2/*c*

Space group (Hall) -C 2yc

Unit cell dimensions  $a = 32.653(2)$  Å

$\alpha = 90^\circ$

$b = 4.8634(4)$  Å

$\beta = 119.984(4)^\circ$

$c = 21.7870(16)$  Å

$\gamma = 90^\circ$

Volume  $2996.8(4)$  Å<sup>3</sup>

Z 8

Calculated density 1.389 Mg/m<sup>3</sup>

Absorption coefficient 0.088 mm<sup>-1</sup>

F(000) 1312

Crystal size 0.890 x 0.070 x 0.040 mm<sup>3</sup>

$\Theta$  range for data collection 2.597 to 28.998°

Index ranges  $-44 \leq h \leq 44$ ,  $-4 \leq k \leq 6$ ,  $-29 \leq l \leq 29$

Reflections collected 20234

Independent reflections 3999 [R(int) = 0.0559]

Completeness to  $\Theta = 28.00^\circ$  99.9%

Absorption correction Multi-scan

Max. and min. transmission 0.7462 and 0.6353

Refinement method Full-matrix least-squares on F<sup>2</sup>

Data / restraints / parameters 2728 / 0 / 219

Goodness-of-fit on F<sup>2</sup> 1.019

Final R indices [ $I > 2\sigma(I)$ ] R1 = 0.0462, wR2 = 0.1076

R indices (all data) R1 = 0.0757, wR2 = 0.1274

Largest diff. peak and hole 0.229 and -0.233 e.Å<sup>-3</sup>

