

Supporting Information

**Design of hybrid heterocyclic systems with furoxanylpyridine core *via* tandem
hetero-Diels–Alder/retro-Diels–Alder reactions of (1,2,4-triazin-3-yl)furoxans**

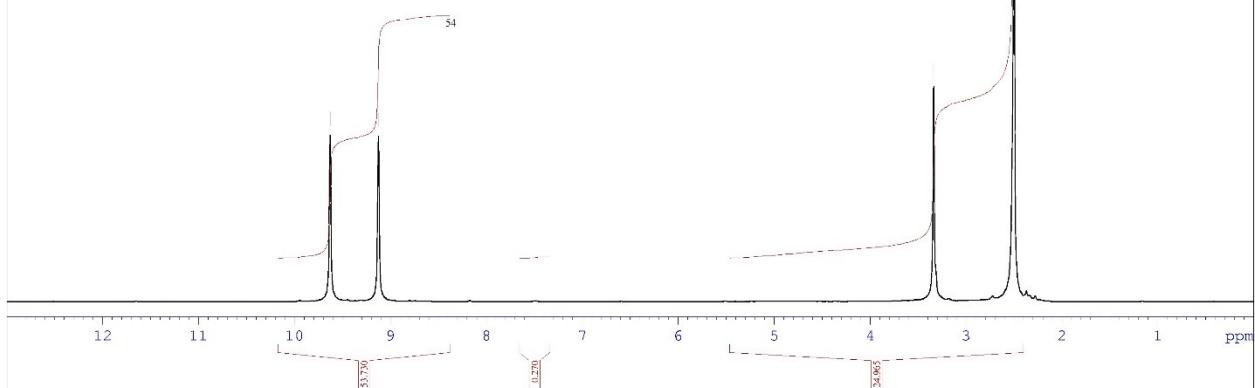
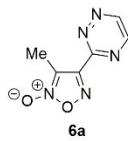
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Alexander S. Kulikov,^a Ivan V. Ananyev,^b Nina. N. Makhova^{a*}

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Moscow, Russian Federation. Fax: +7 499 135 53 28. E-mail: mnn@ioc.ac.ru

^b A.N. Nesmeyanov Institute of Organoelement Compounds, Vavilova str. 28,
119991 Moscow, Russian Federation.

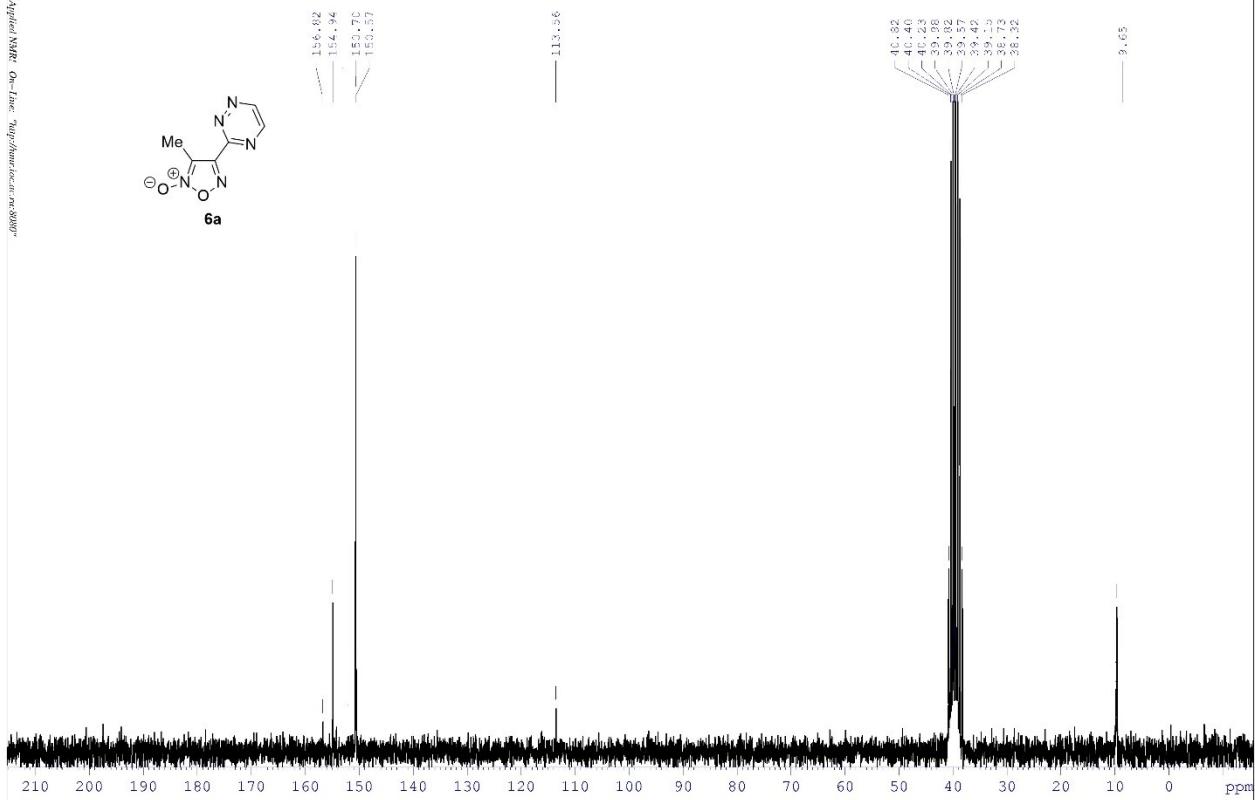
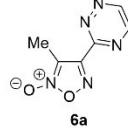
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=16K SW=7500 O1=2200 PW=9.0 AQ=1.082 RD=2.00 NS=1 SR=1.82 TE=300K 17 April 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; NMR/50095095

The Best Applied NMR: On-Line: <http://nmr.zin.rssi.ru/nmr50095095>

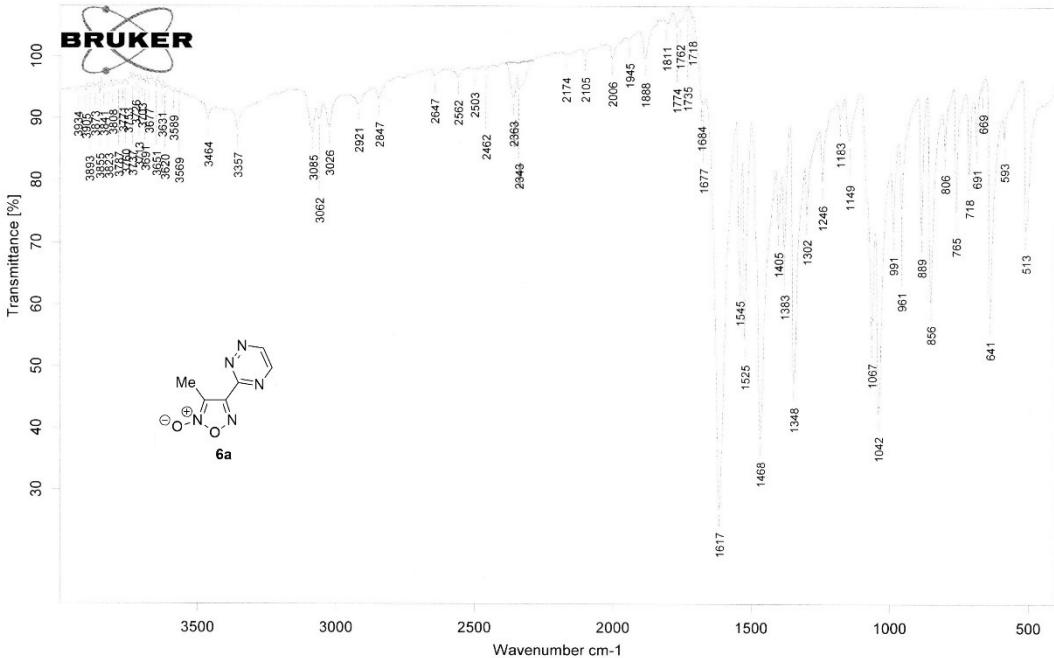


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AC200 SF=50.32 MHz {¹³C} SI=1627 O1=5600 PW=6.0 AQ=0.705 RD=2.00 NS=21618 SR=378.20 T2=297K 29 December 2015 Opr: Struchkova M.I.; Solv:DMSO-d₆; /USED D7A.C13

The Best Applied NMR: On-Line: <http://nmr.zin.rssi.ru/nmr50095095>



¹³C NMR (50.3 MHz, DMSO-d₆) of **6a**



D:\MED\LEO-L48.0 ФЕРШТАТ LEO-L48 прессовка с KBr 1/200.

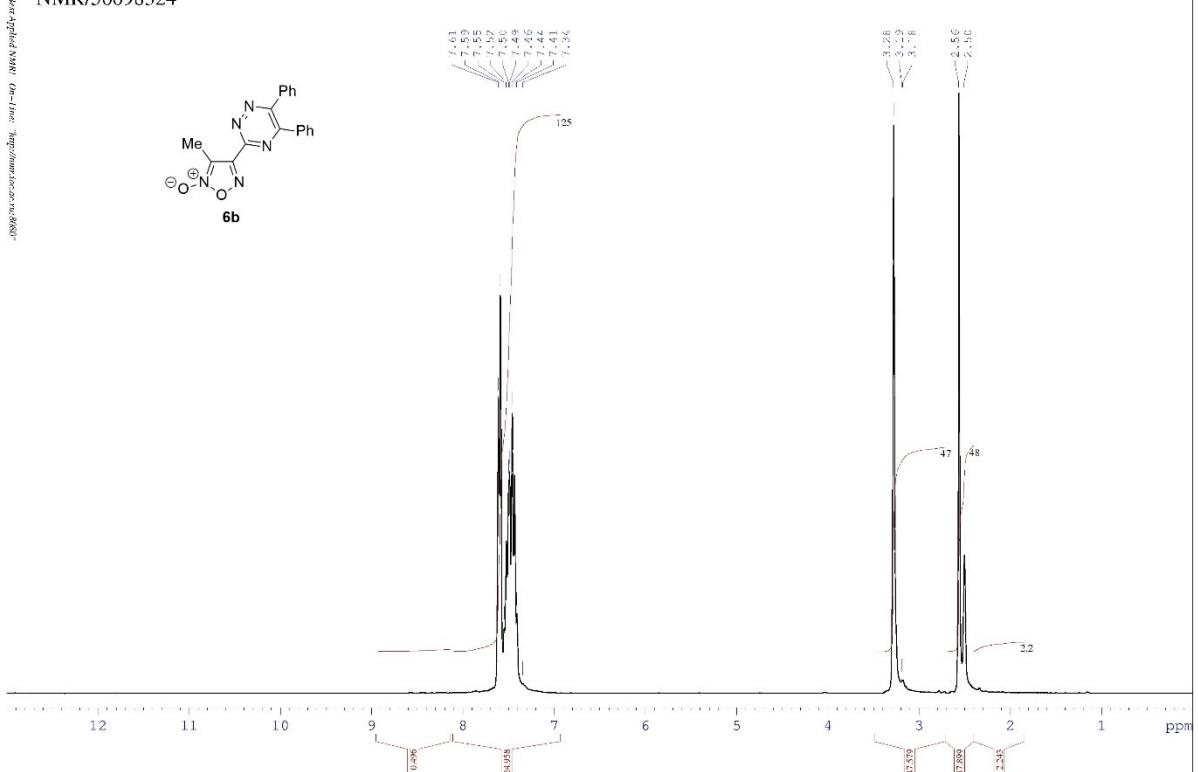
13.11.2015

Ране 1/1

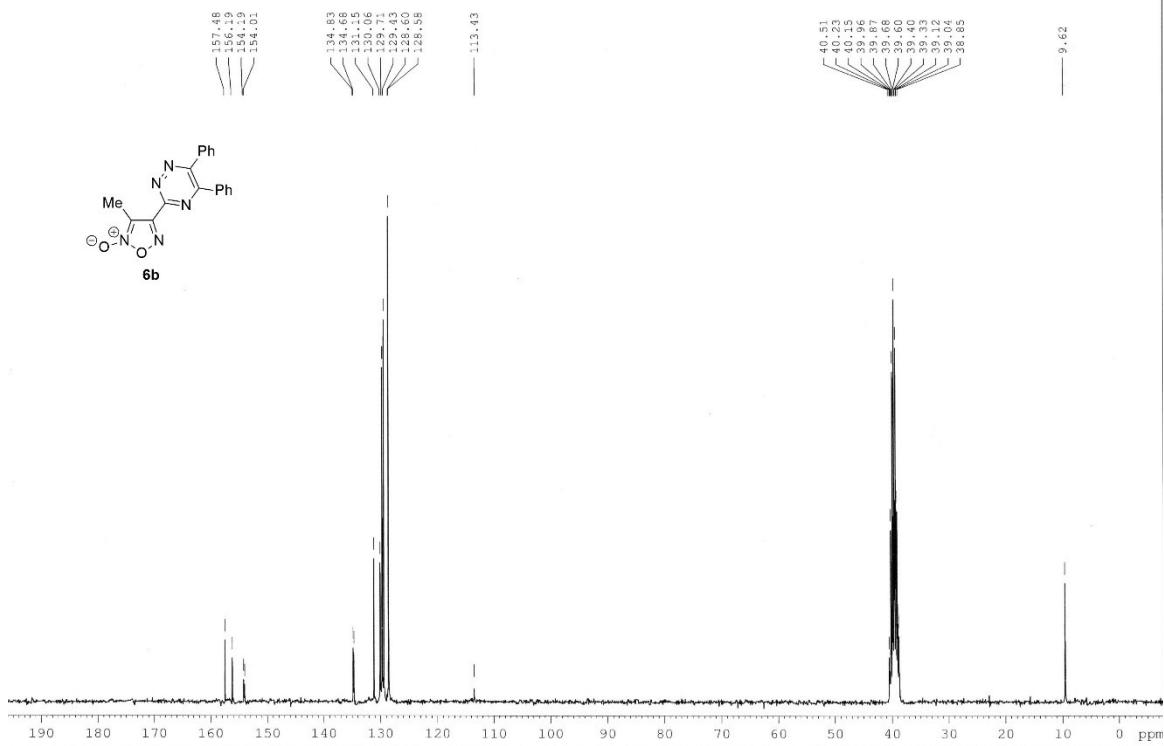
IR (KBr) of **6a**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300, SF=300, 13 MHz {¹H}; SI=16K SW=7500 O Δ=2200 PW=9.0 AQ=1.082 RD=3.00 NS=1 SR=4.83 TP=300K 12 May 2015 Opt: Struchkova M.L.; Solv: DMSO-d₆;

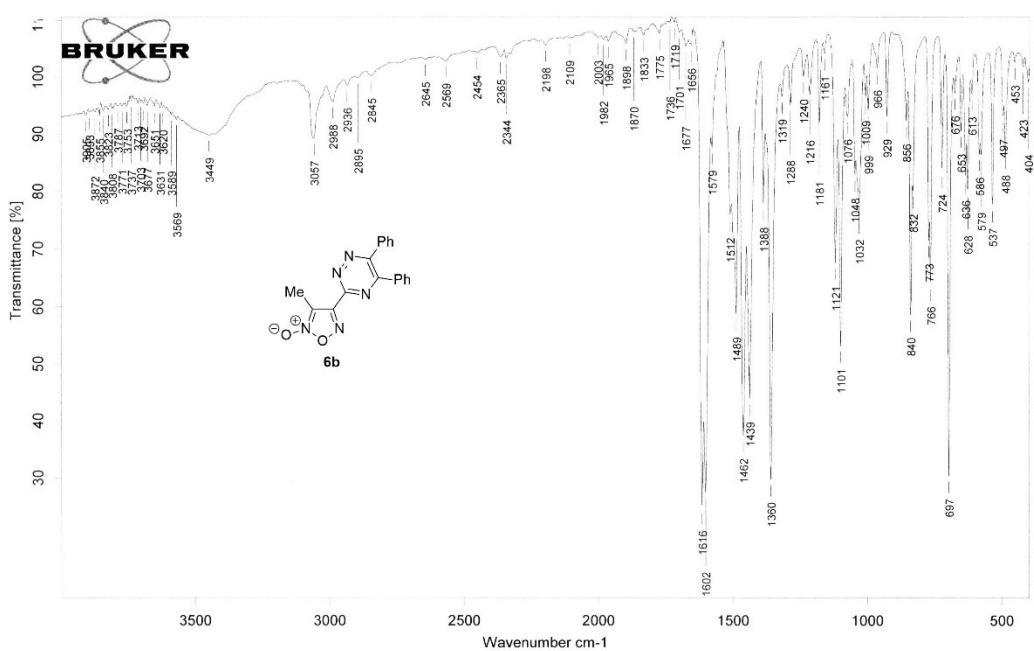
NMR/50098324



¹H NMR (300 MHz, DMSO-d₆) of **6b**



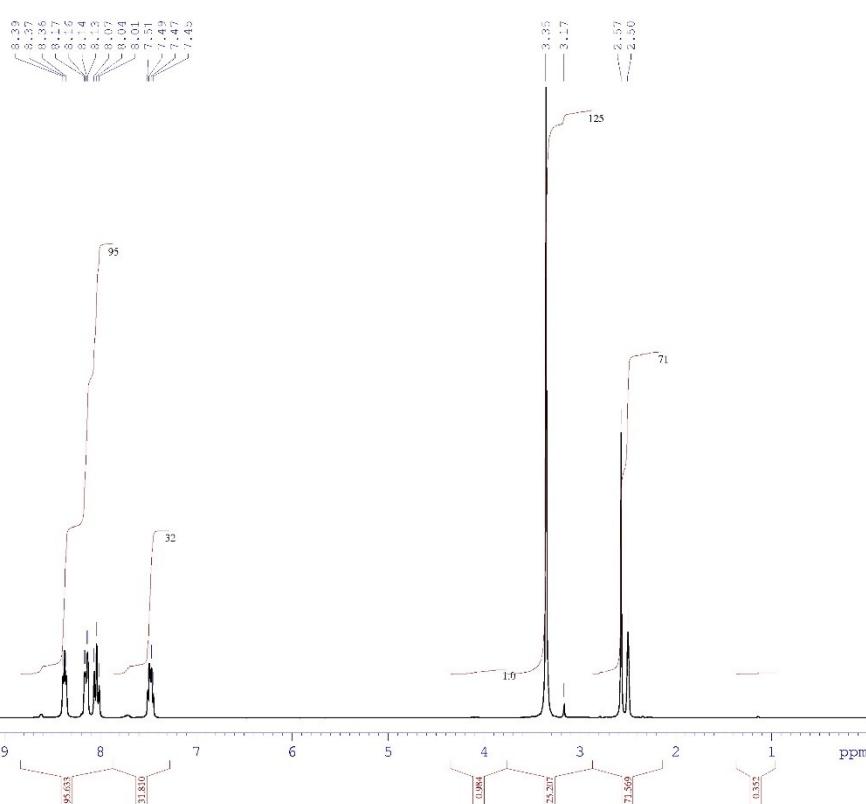
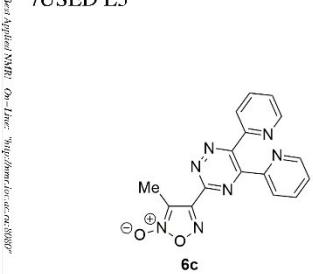
^{13}C NMR (75.5 MHz, DMSO-d₆) of **6b**



D:\EDL\378.0 ЕПИШНА. 378 , прессовка с KBr, 1/200.

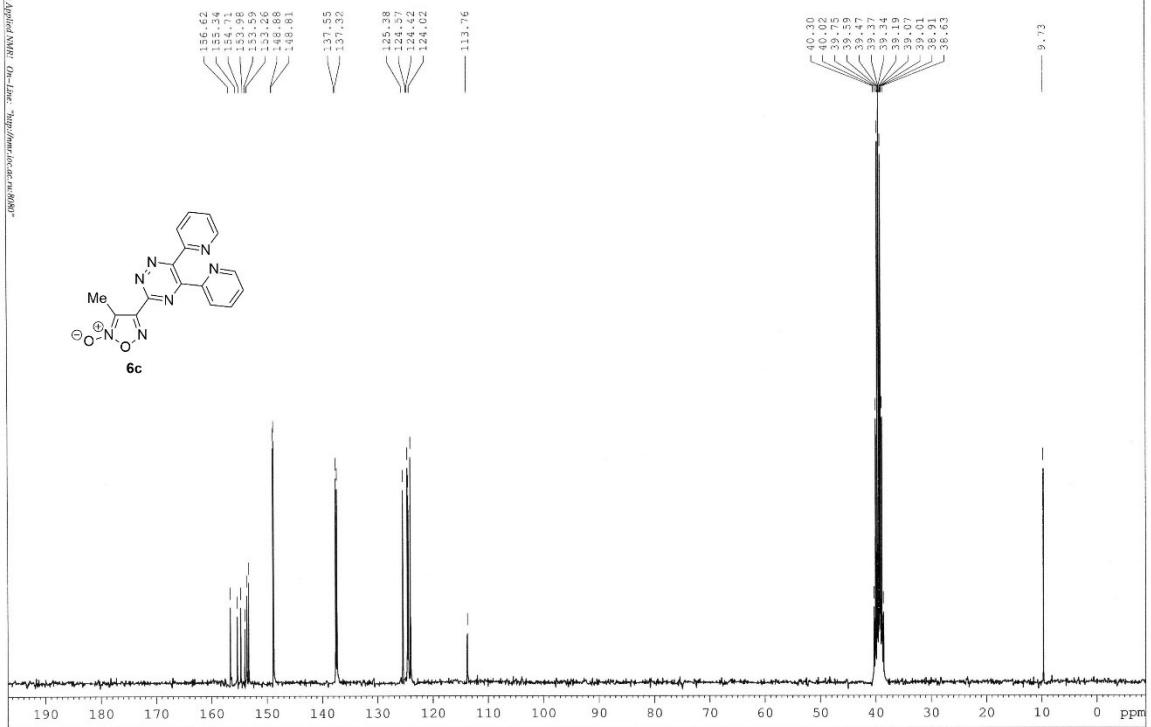
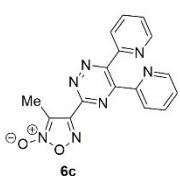
12.11.2015

USED L3

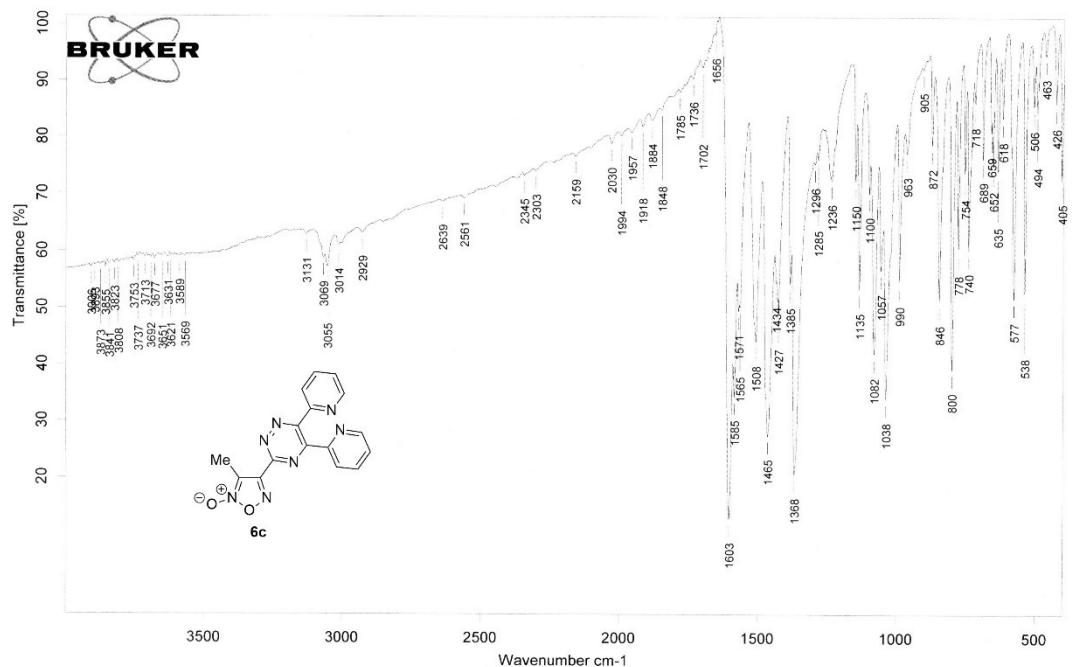


¹H NMR (300 MHz, DMSO-d₆) of **6c**

1 USED 853



¹³C NMR (75.5 MHz, DMSO-d₆) of **6c**



D:\EDL\LEO-853.0 ФЕРШТАТ. LEO-853 . прессовка к KBr. 1/200

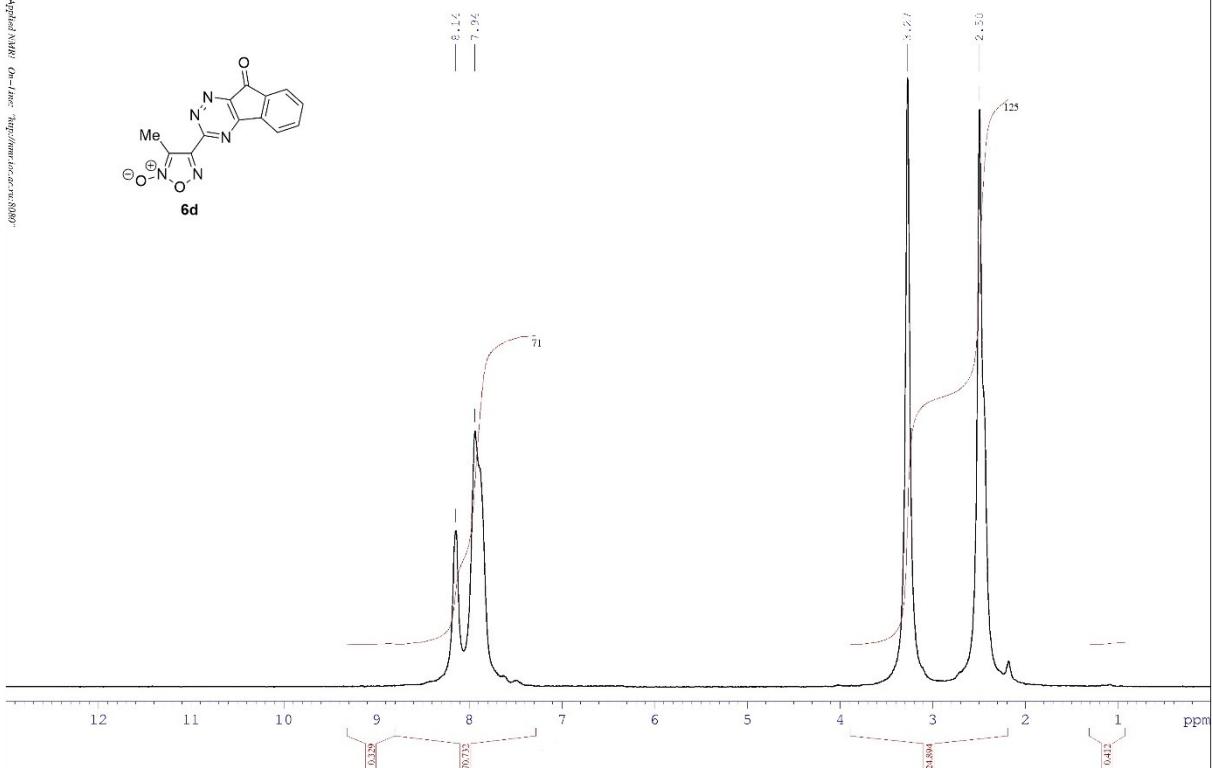
13.11.2015

Page 1/1

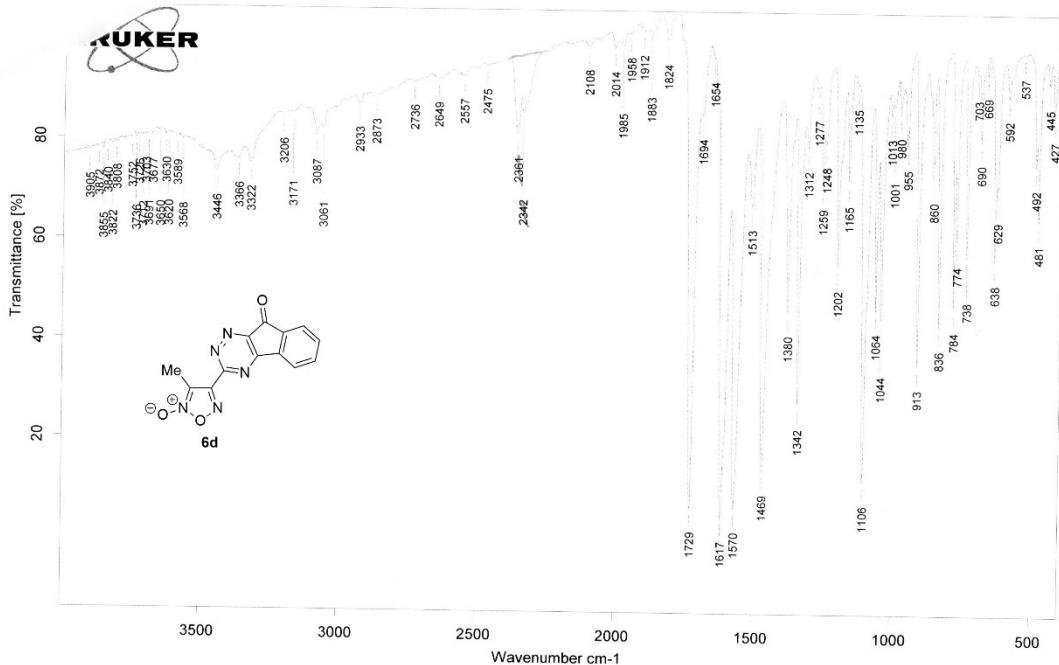
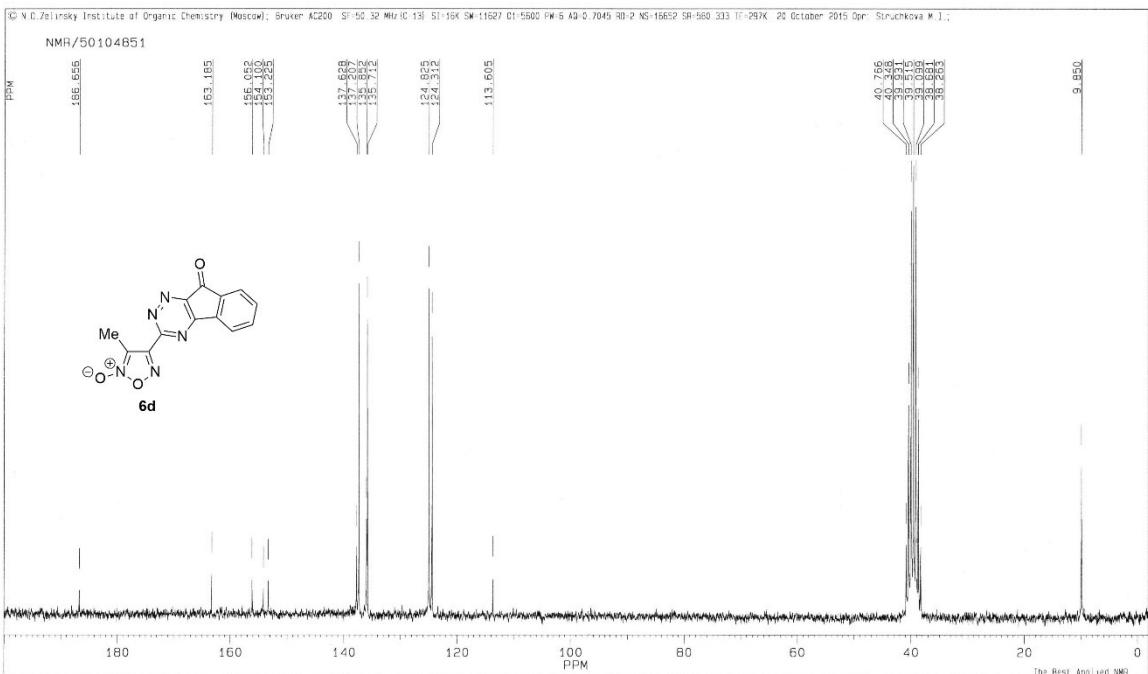
IR (KBr) of **6c**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H}; Sl=16K SW=7500 O1=2200 PW=0.0 AQ=1.082 RD=3.00 NS=1 SR=19.56 TE=299K 16 October 2015 Oper: Struchkova M.I.; Solv: DMSO-d6;

NMR/50104851



^1H NMR (300 MHz, DMSO- d_6) of **6d**



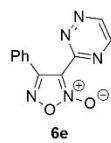
D:\EDL\352.0 ЕПИШИНА_352_прессовка с KBr.1/200

29.10.2015

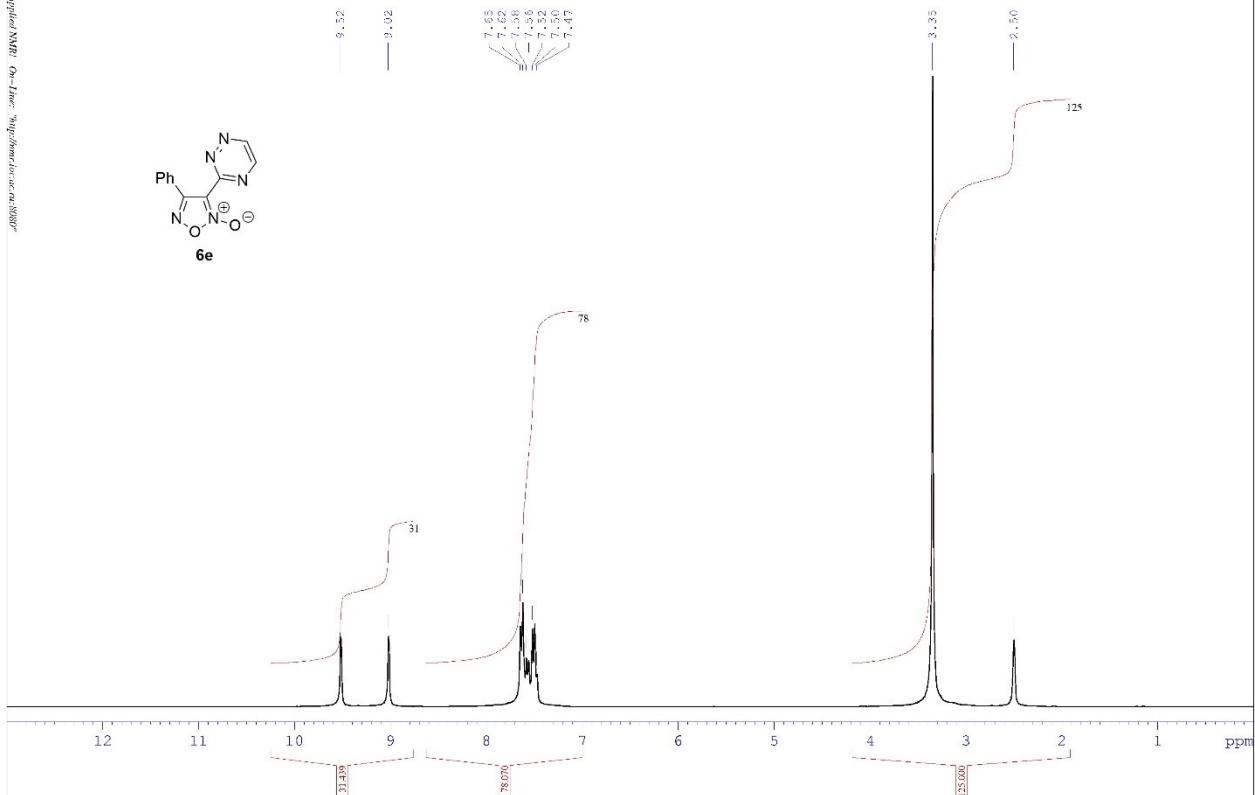
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=16K SW=7500 O1=2200 PW=9.0 AQ=1.082 RD=3.00 NS=1 SR=1.55 TE=301K 5 November 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED MA388/

/USED MA388/

The Best Applied NMR. On-Line. <http://www.mercklin.ac.ru/388/>



6e

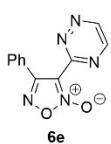


¹H NMR (300 MHz, DMSO-d₆) of **6e**

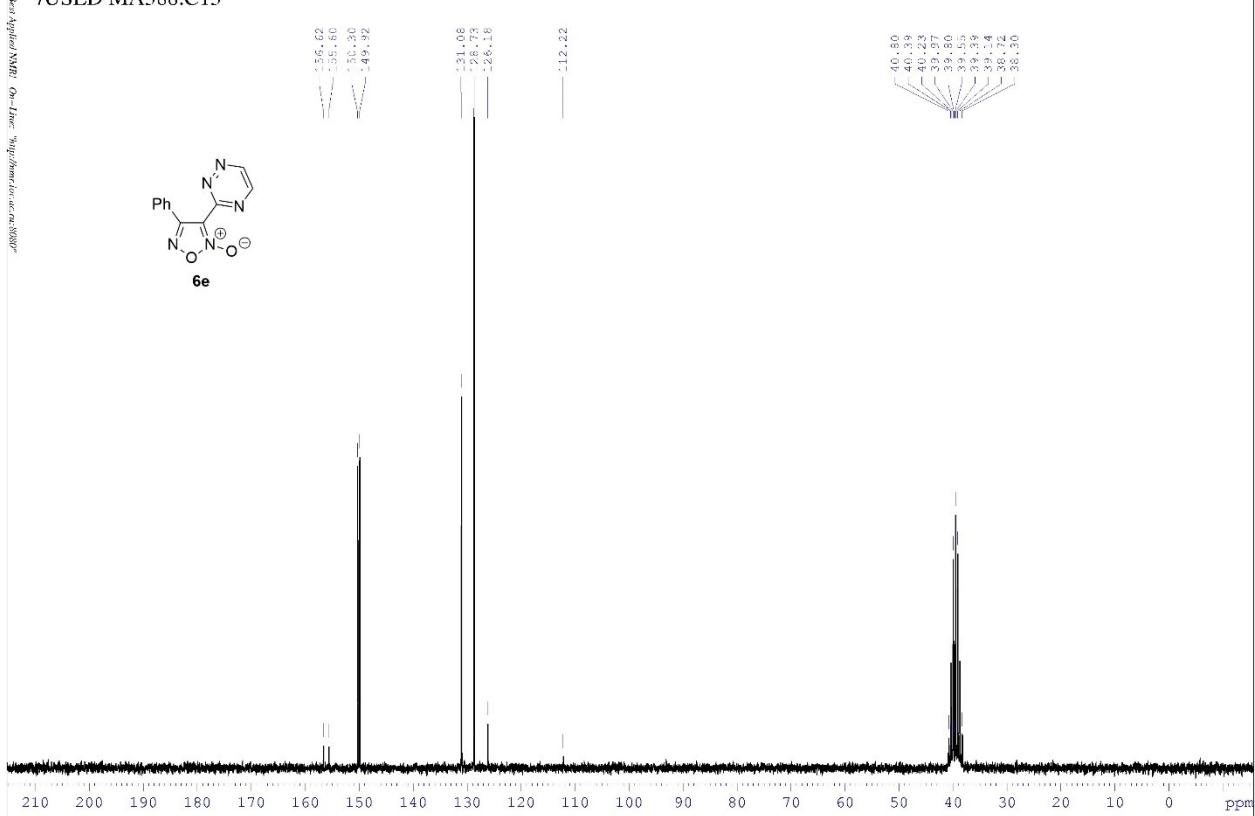
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AC200 SF=50.32 MHz {¹³C} SI=16K SW=11627 O1=5600 PW=6.0 AQ=0.705 RD=2.00 NS=15940 SR=378.20 TE=297K 6 November 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED MA388.C13/

/USED MA388.C13/

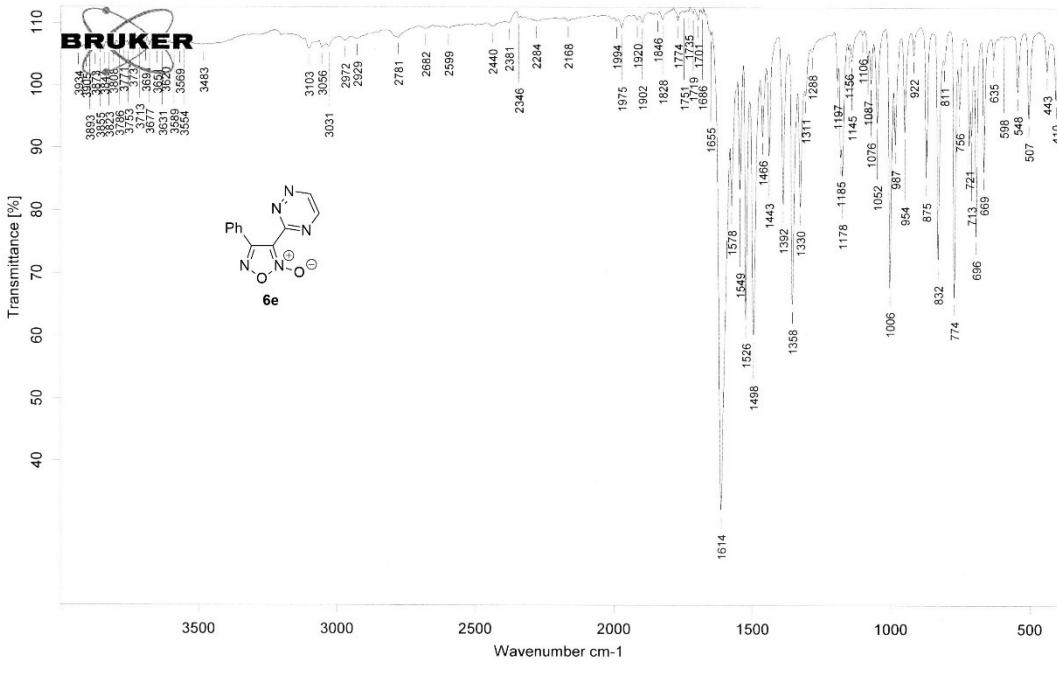
The Best Applied NMR. On-Line. <http://www.mercklin.ac.ru/388/>



6e



¹³C NMR (50.3 MHz, DMSO-d₆) of **6e**



D:\EDL\MA-388.0 ФЕРШТАТ. MA-388 , прессовка с KBr, 0,5/200

19.11.2015

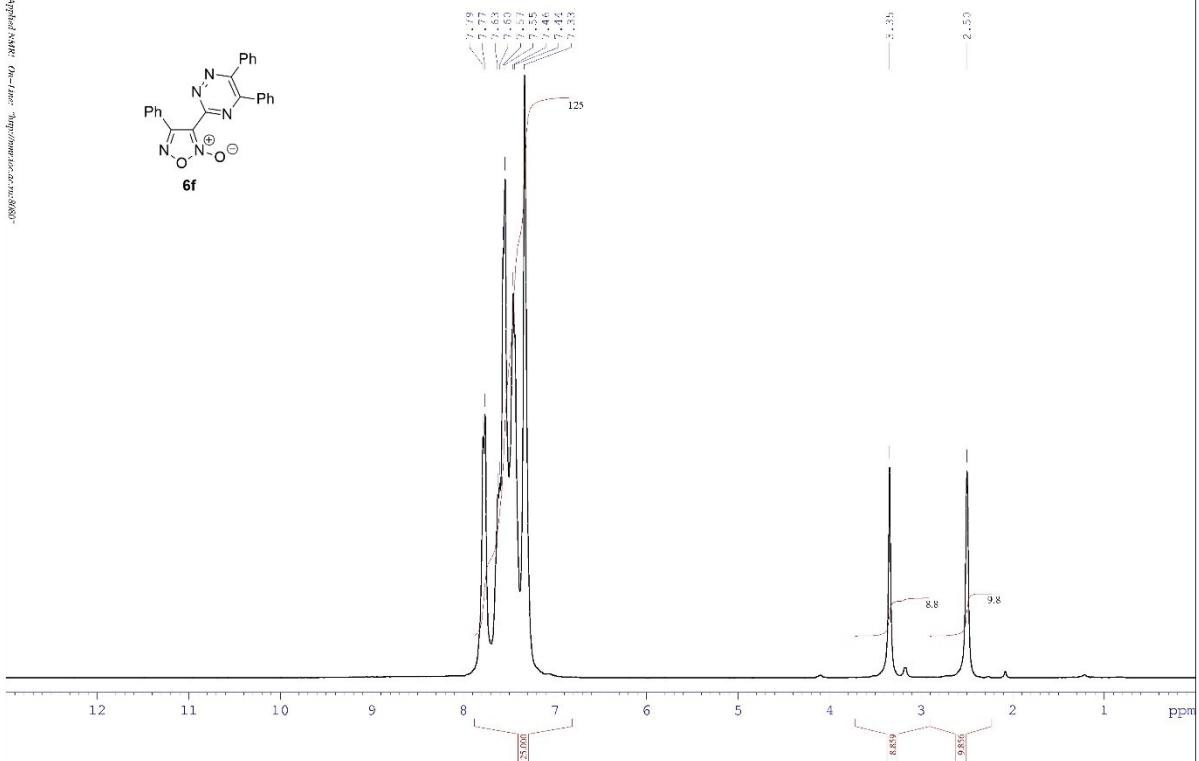
Page 1/1

IR (KBr) of **6e**

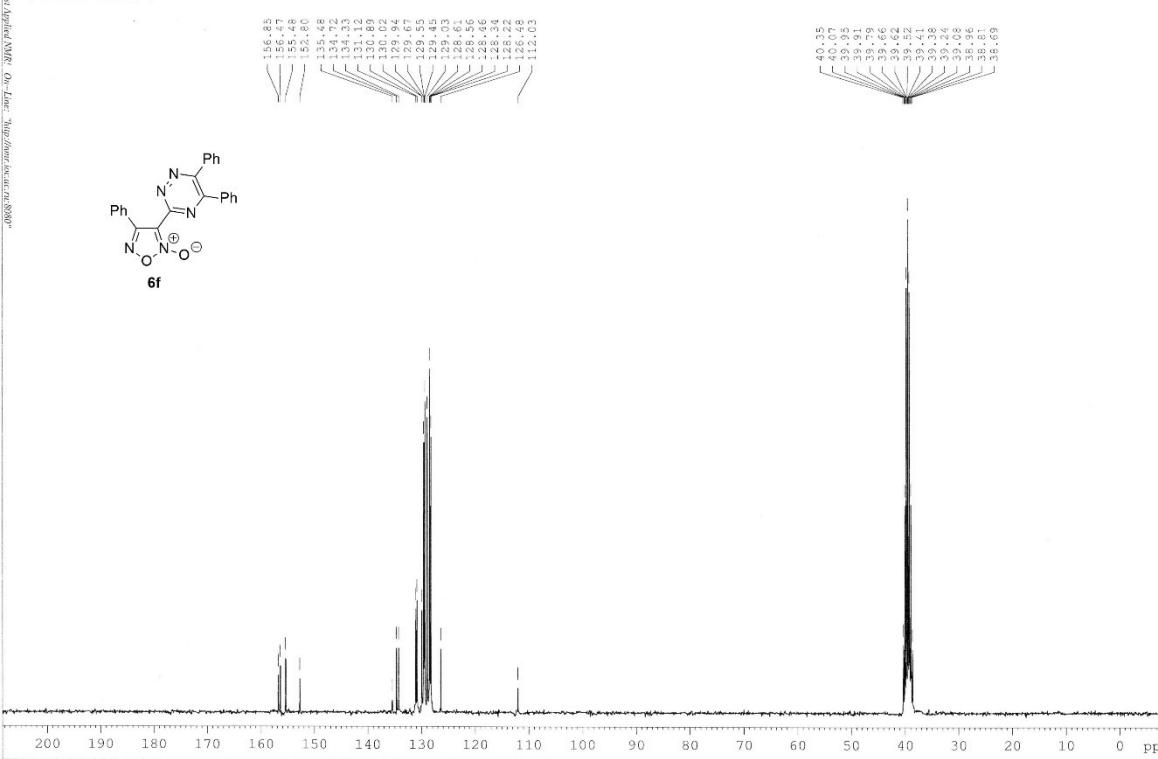
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM390 SF=390.13 MHz {¹H} SI=16K SW=7500 O=2200 PW=9.0 AQ=1.082 RD=3.06 NS=1 SR=1.55 TP=297K 16 November 2015 Opt: Struchkova M.I.; Solv: DMSO-d₆;

/USED ma390

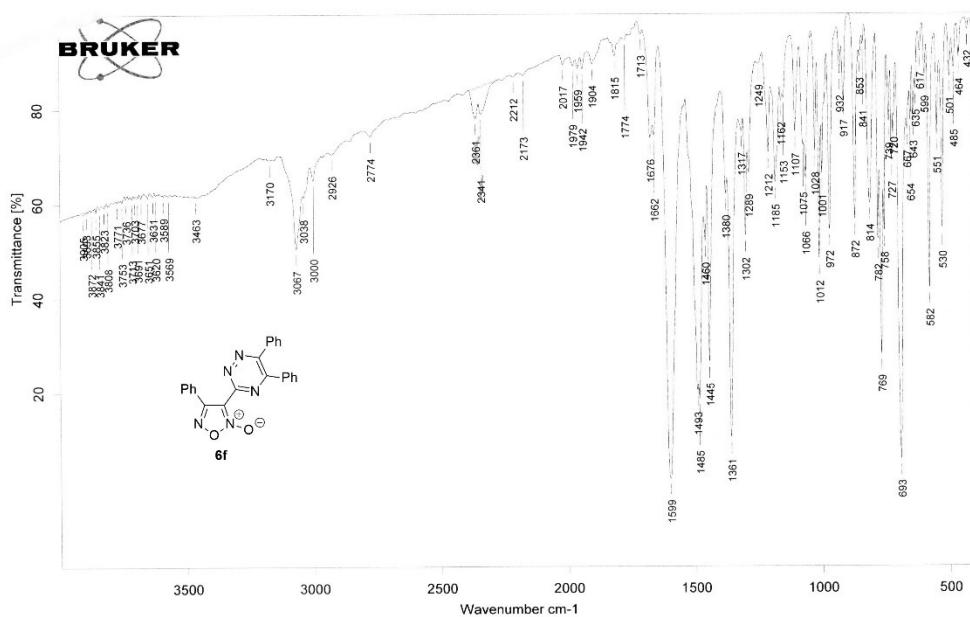
The Best Applied NMR - On-Line: http://onlinenmr.scs.ru/8085



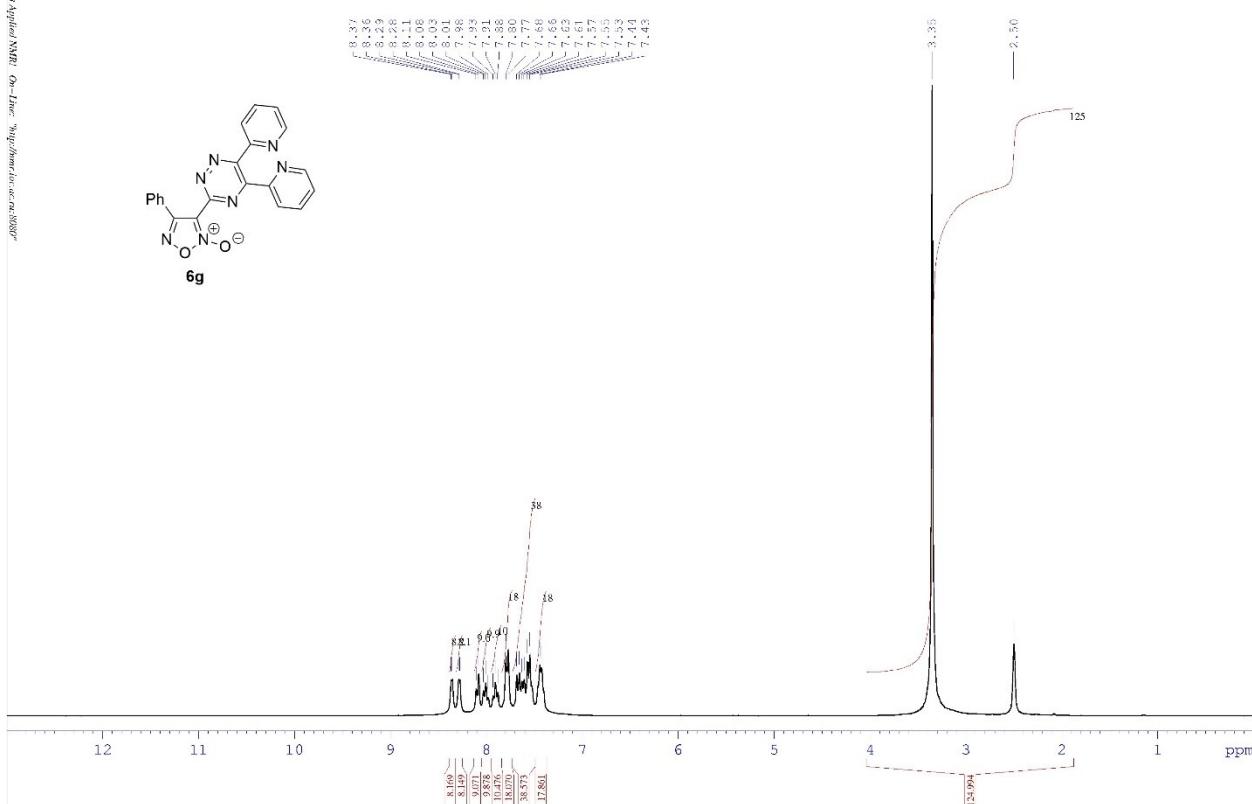
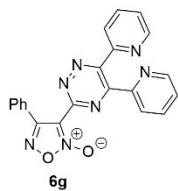
¹H NMR (300 MHz, DMSO-d₆) of **6f**



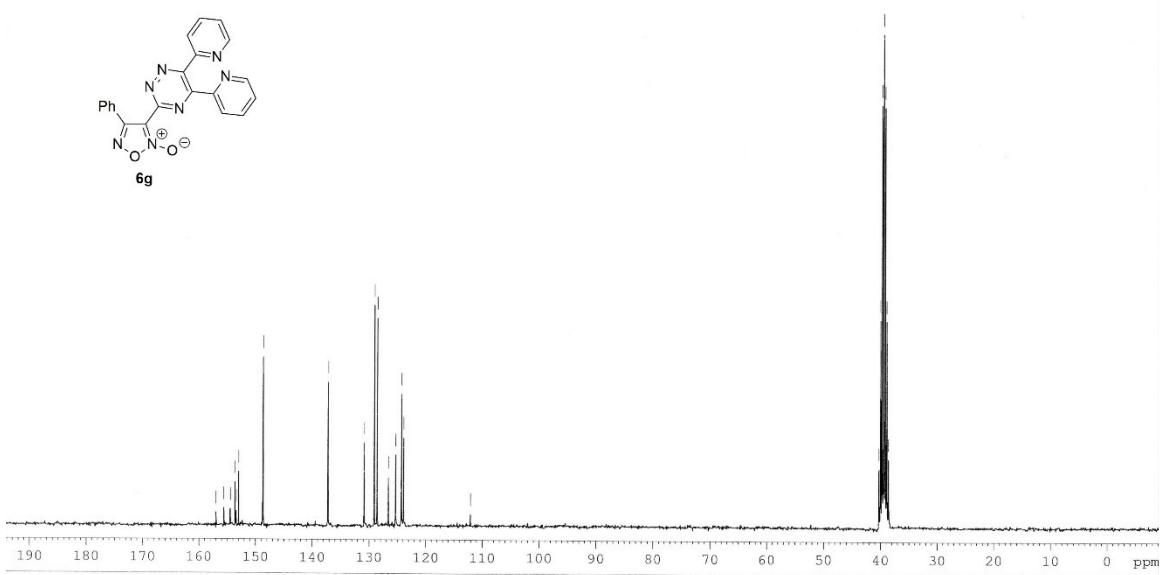
¹³C NMR (75.5 MHz, DMSO-d₆) of **6f**



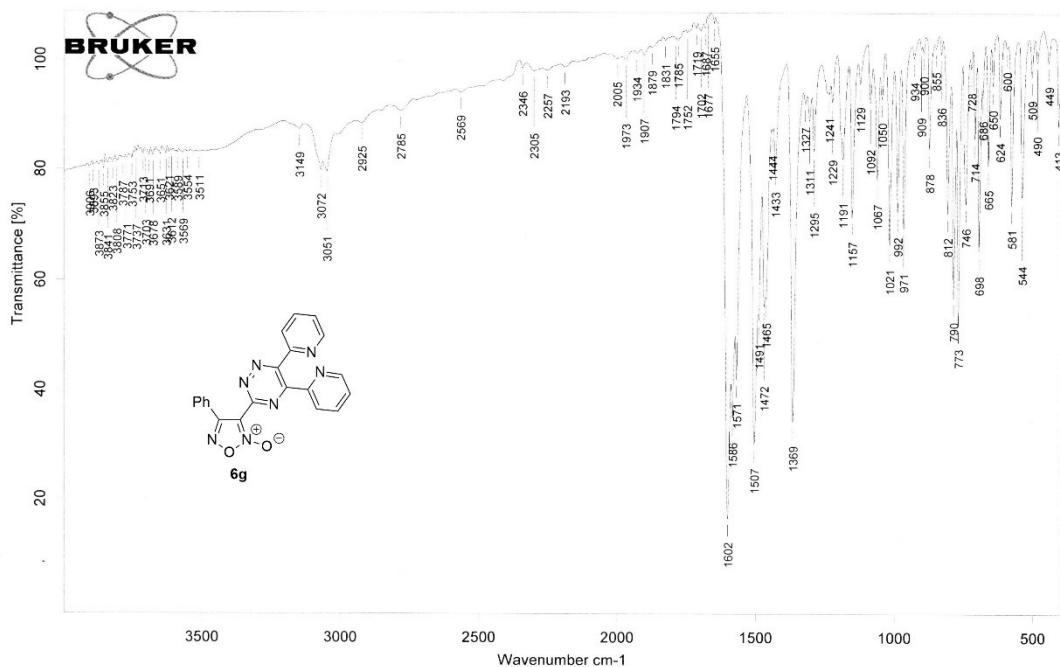
The Best Applied NMR: On-Line: <http://www.jmr.msu.ru/nmr/> Date: 2020-07-07



¹H NMR (300 MHz, DMSO-d₆) of 6g



¹³C NMR (75.5 MHz, DMSO-d₆) of 6g



D:\EDLIMA-389.0 ФЕРШТАТ. МА-389, прессовка с KBr, 0.5/200

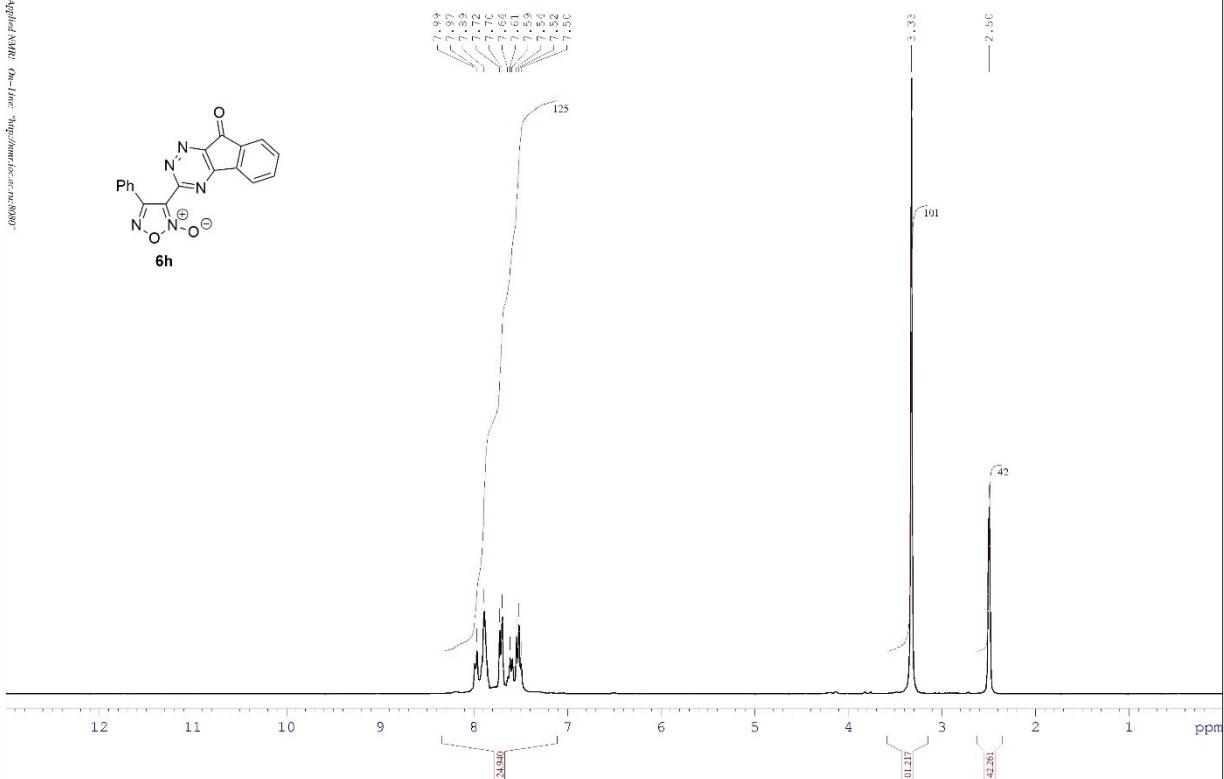
19.11.2015

Page 1/1

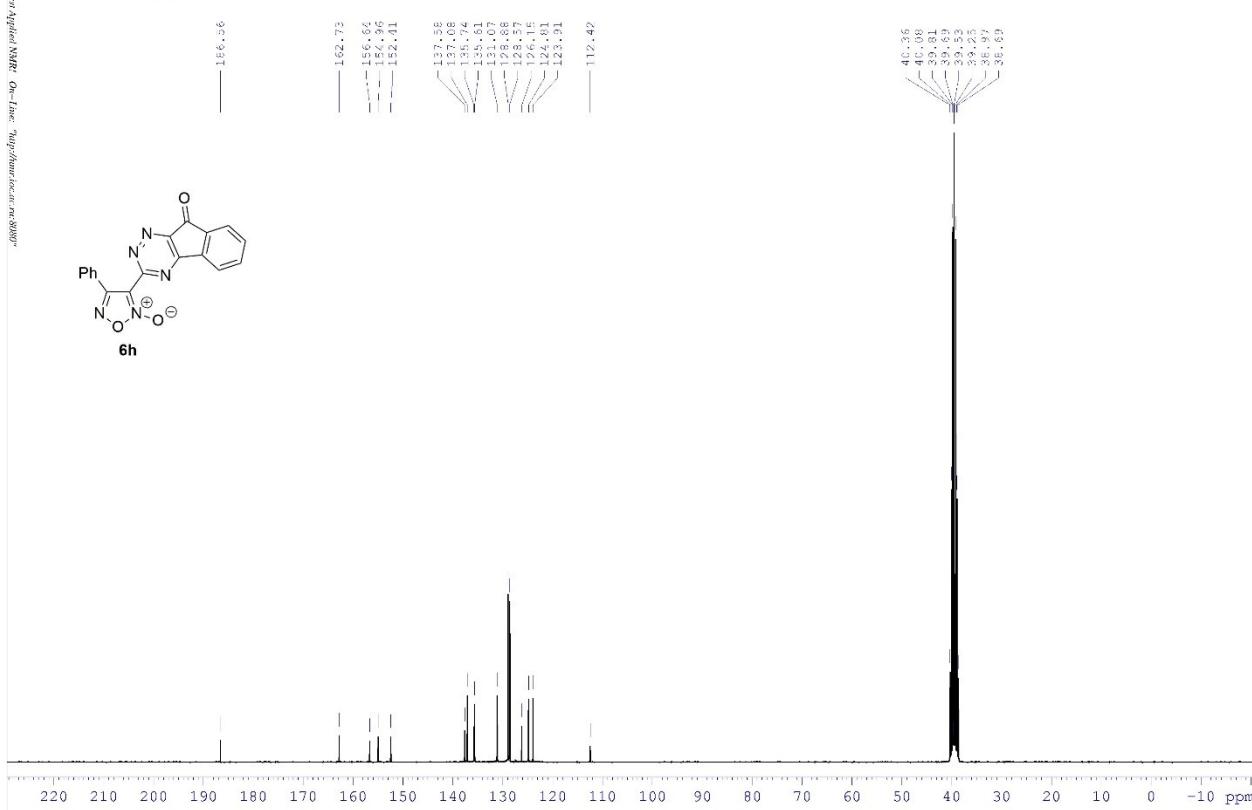
IR (KBr) of 6g

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H}; SI=16K SW=90.09 O1=2200 PW=9.0 AQ=0.901 RD=3.00 NS=1 SR=4.55 TE=298K 11 December 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED L68

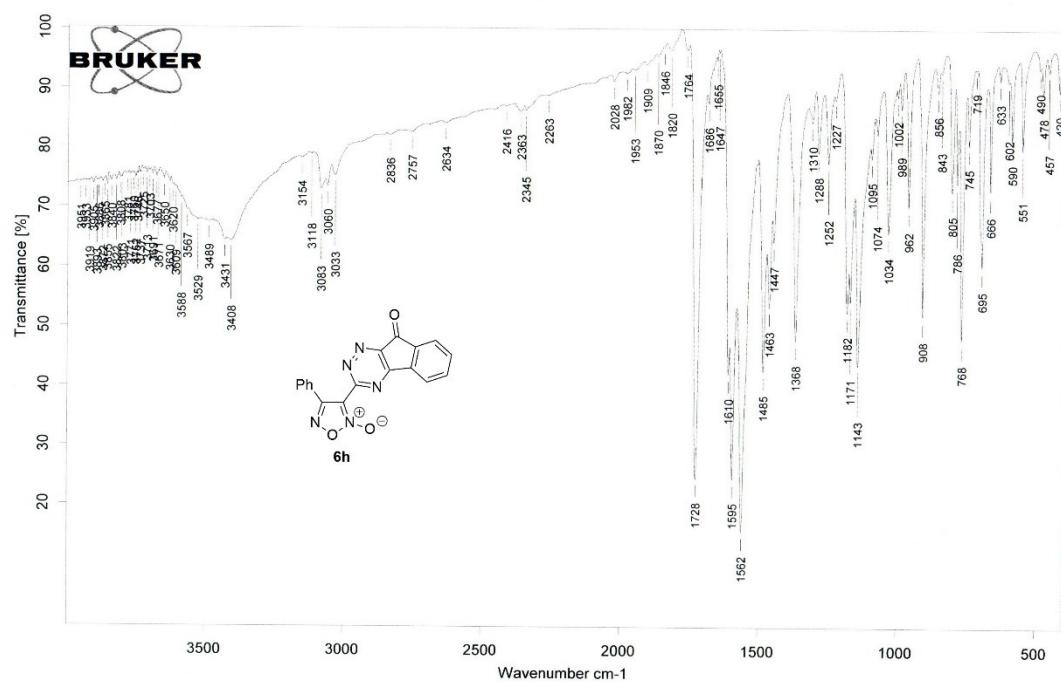
The Best Applied NMR On-Line: <http://nmp.zin.rssi.ru>



¹H NMR (300 MHz, DMSO-d₆) of 6h



¹³C NMR (75.5 MHz, DMSO-d₆) of **6h**

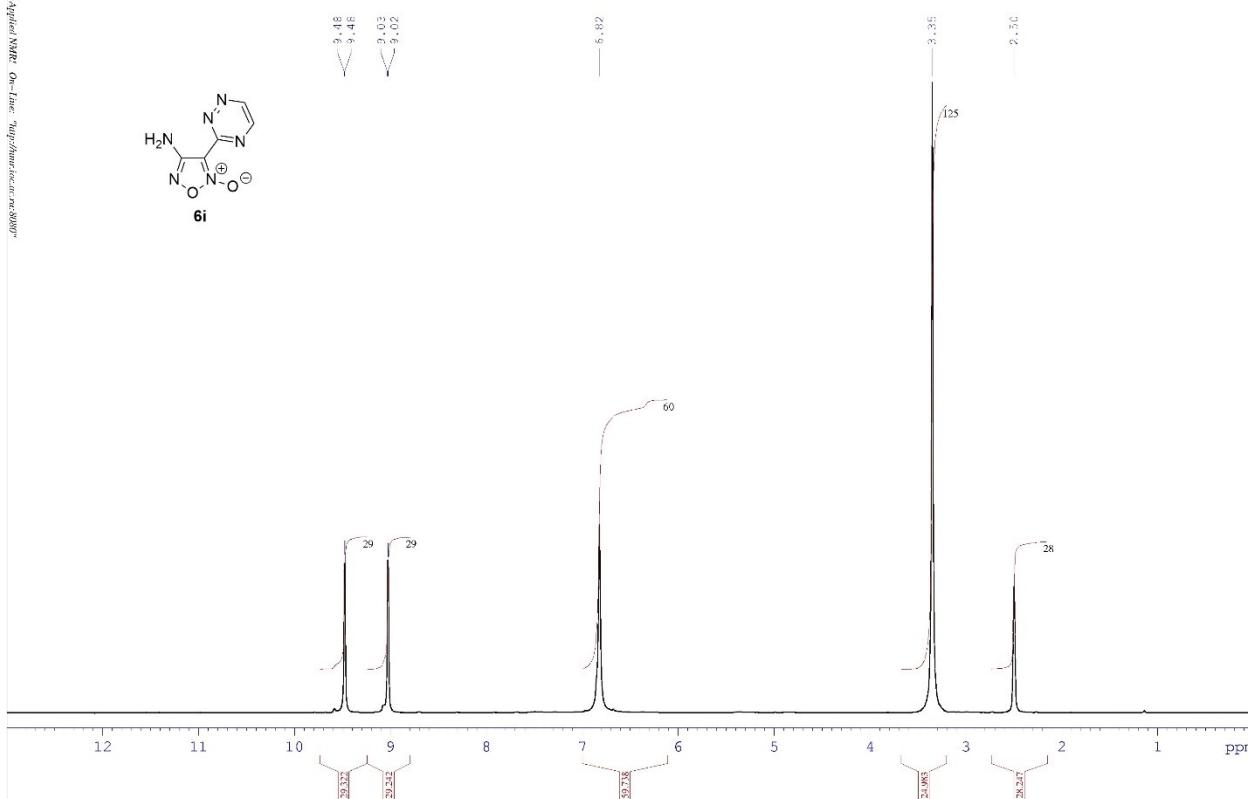


D:\EDL\LEO-L107.0 ФЕРШТАТ. LEO-L107, прессовка с KBr, 1/200.

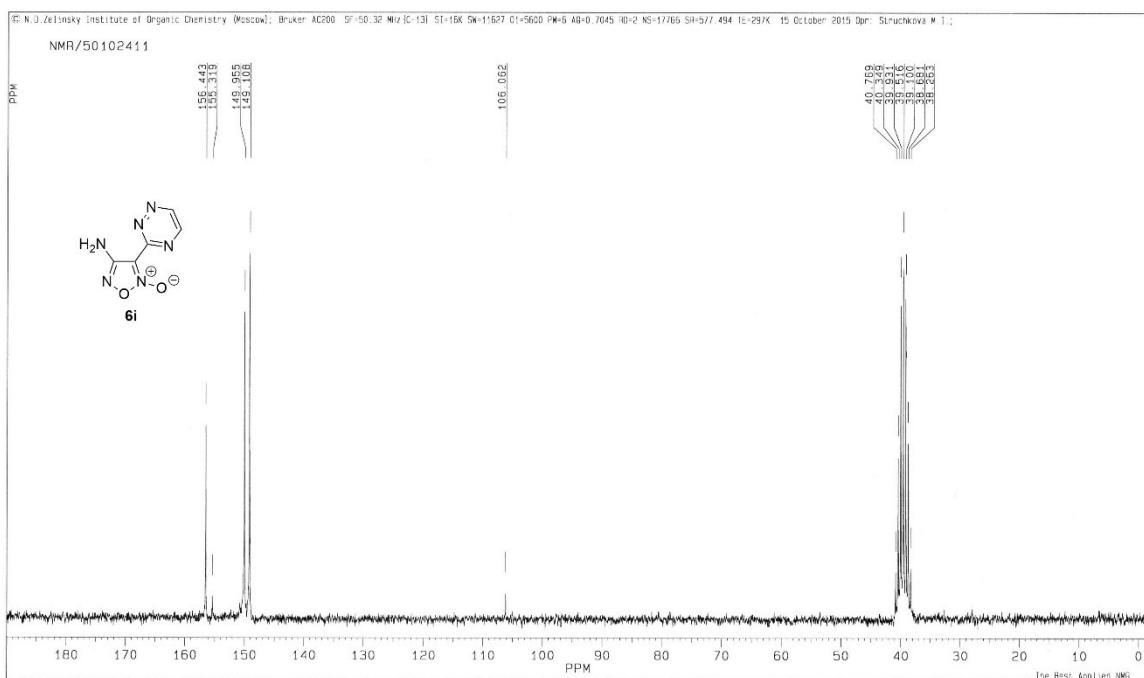
18.01.2016

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=16K SW=7500 O1=2200 PW=9.0 AQ=1.082 RD=3.00 NS=1 SR=1.55 TE=299K 13 October 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; NMR/50102411

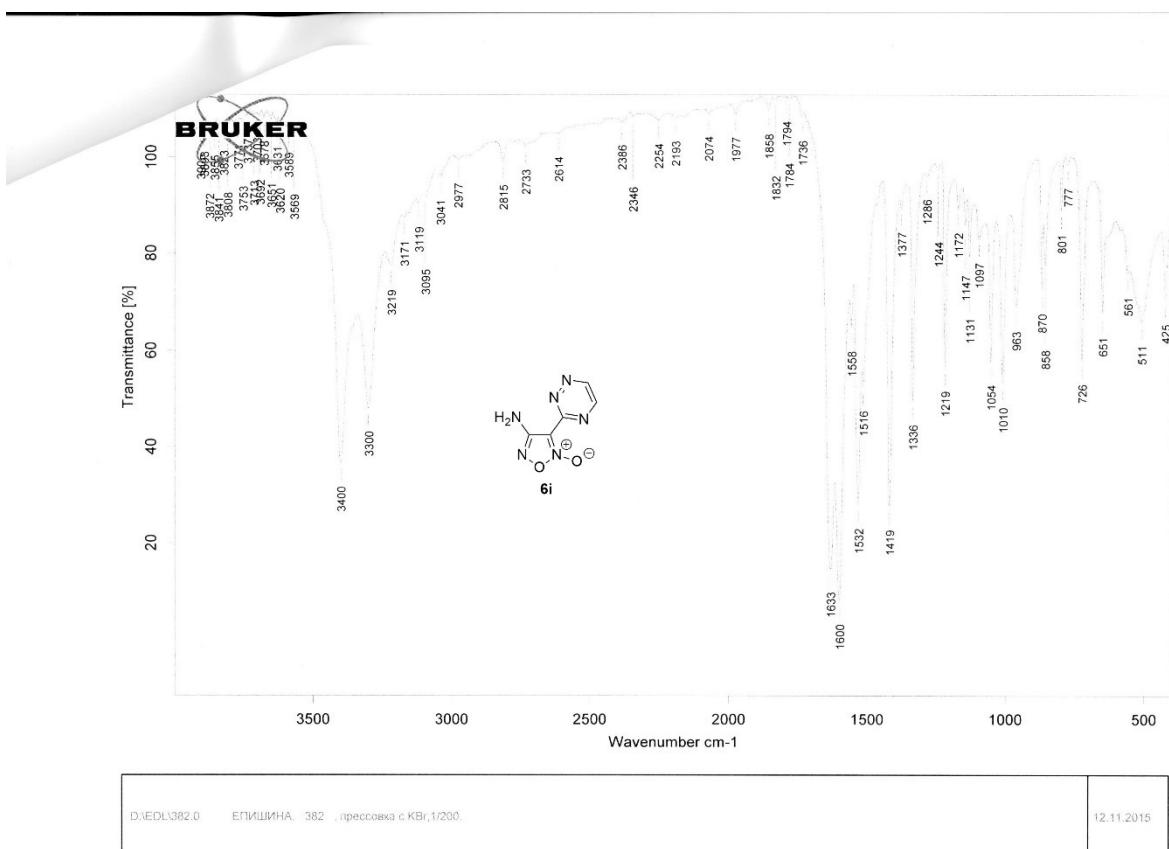
The Best Applied NMR On-Line: <http://www.nmr.ac.ru/nrc3000/>



¹H NMR (300 MHz, DMSO-d₆) of **6i**



¹³C NMR (50.3 MHz, DMSO-d₆) of **6i**



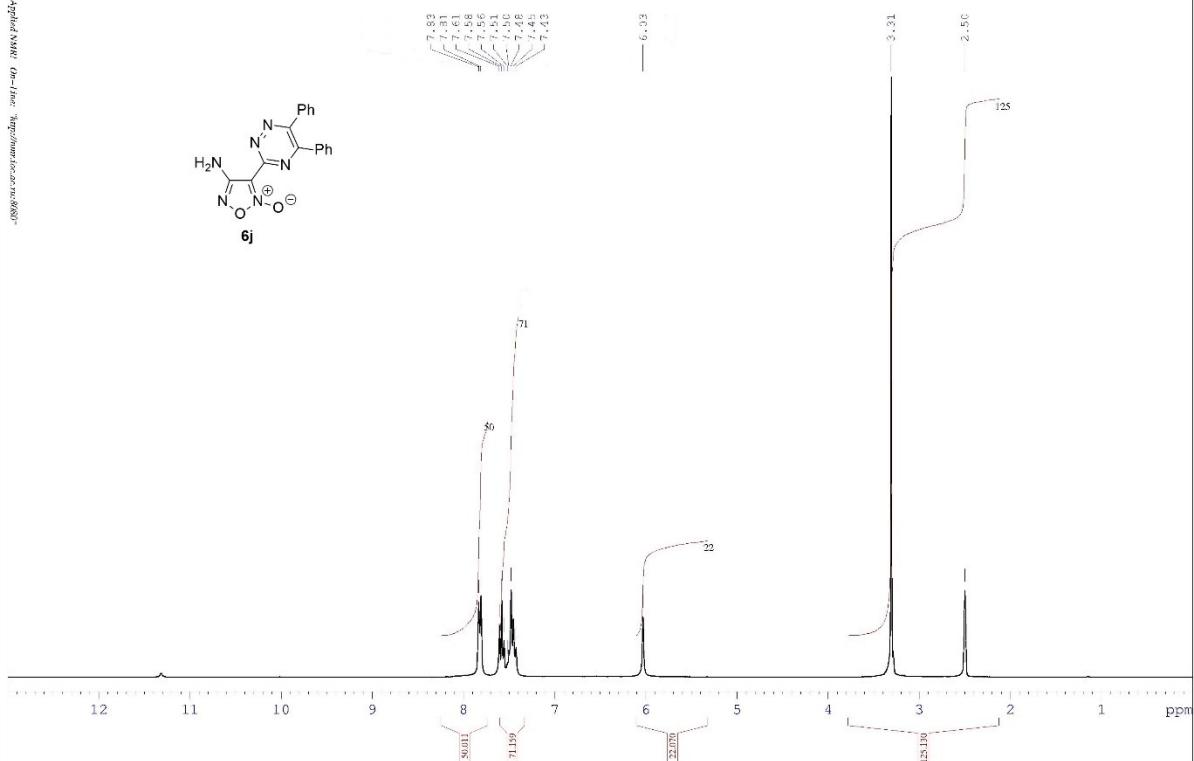
D:\EDL\382.0 ЕПИШИНА_382_прессовка с KBr, 1/200.

12.11.2015

Page 1/1

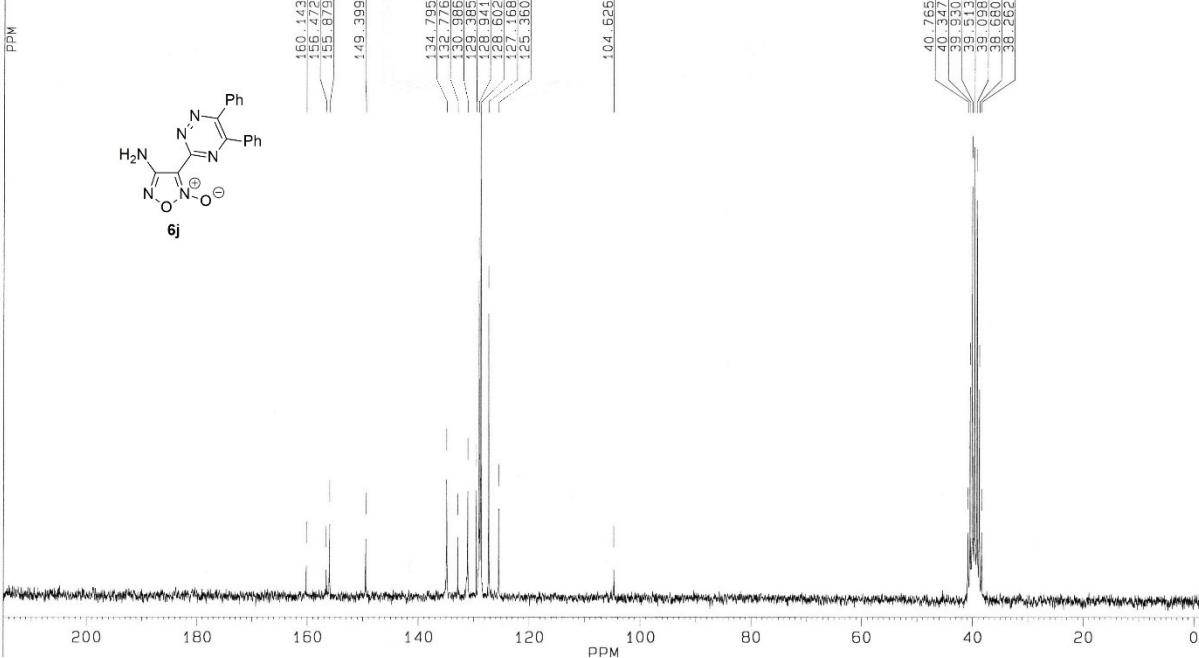
IR (KBr) of **6i**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SP=300.13 MHz {¹H}; Sl=16K SW=7500 O=a2200 PW=9.0 AQ=1.082 RD=3.00 NS=1 SR=1.55 TP=307K 20 October 2015 Opt: Strachikova M.L.; Solv: DMSO-d₆; NMR/50104031

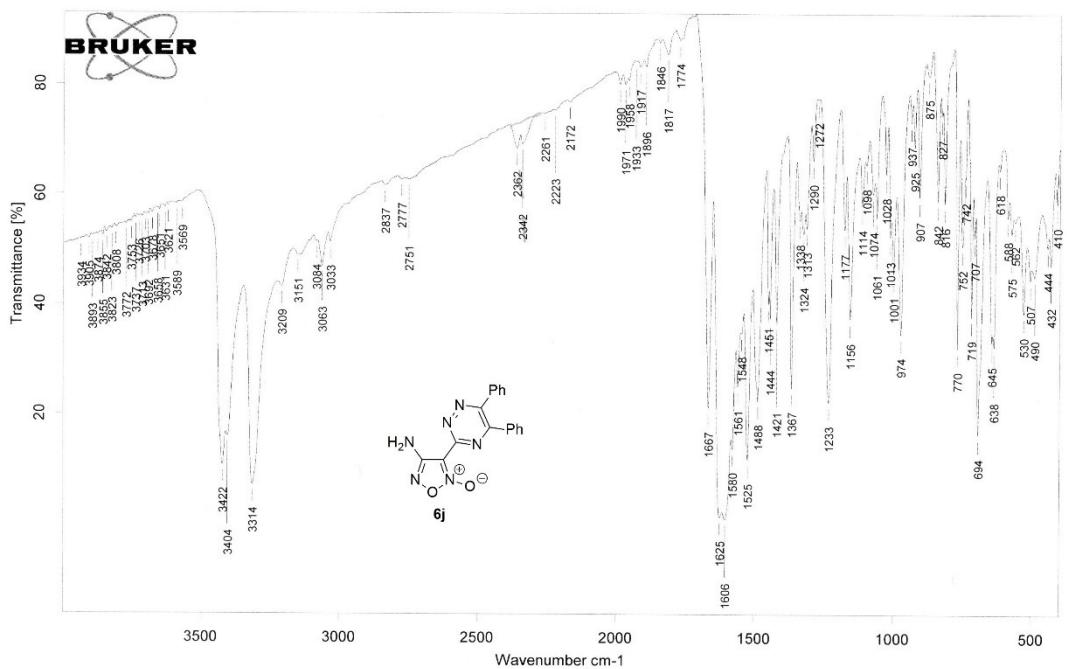


¹H NMR (300 MHz, DMSO-d₆) of **6j**

NMR/50104031

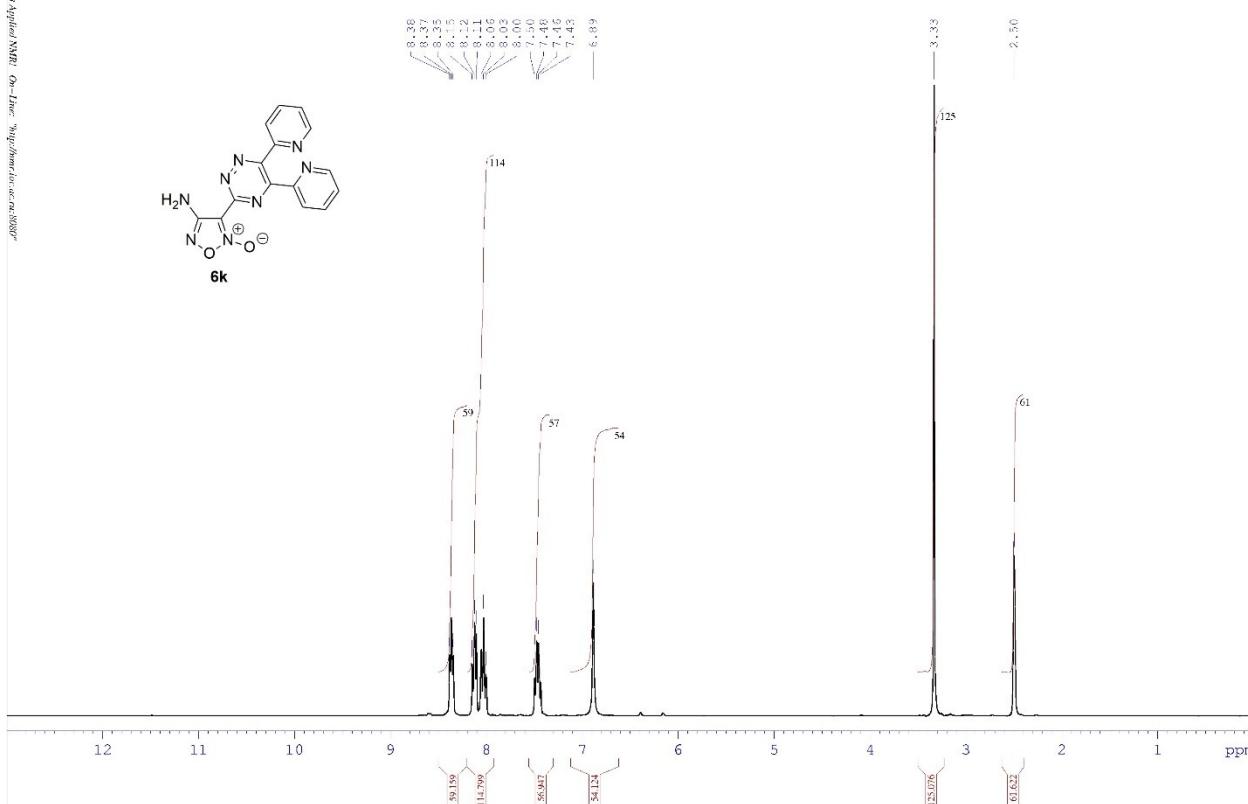


¹³C NMR (50.3 MHz, DMSO-d₆) of **6j**

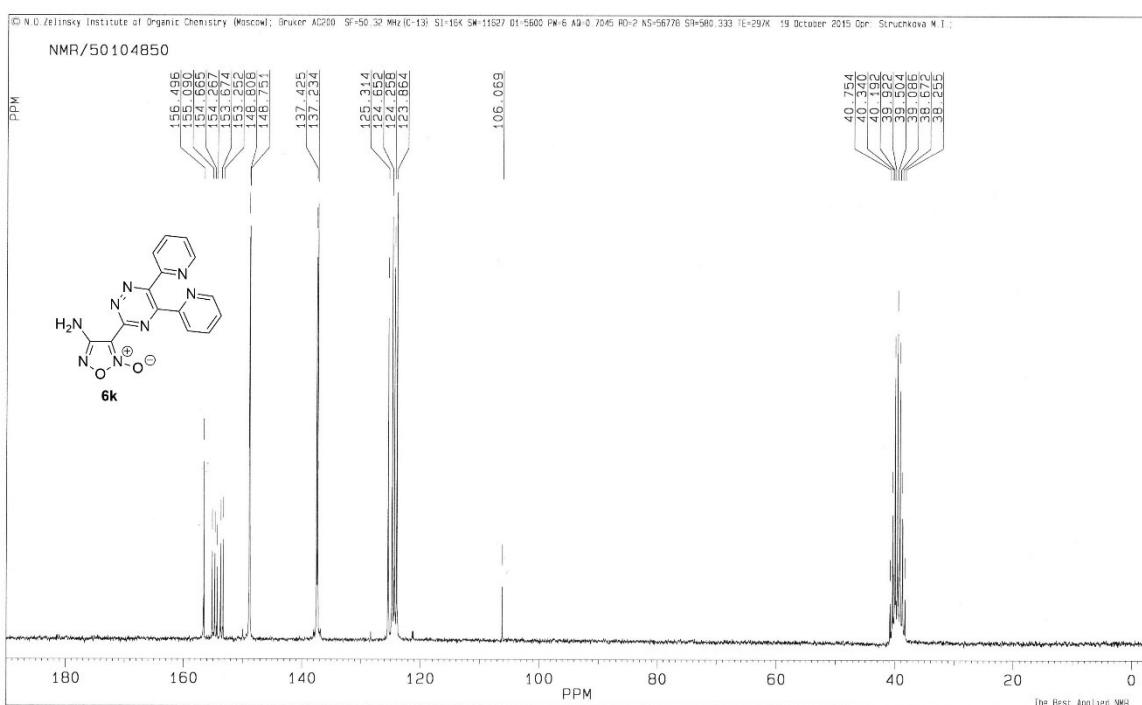


D:\EDL\LEO-MA383.0 ФЕРШТАТ. LEO-MA383 .прессовка с KBr,1/200.

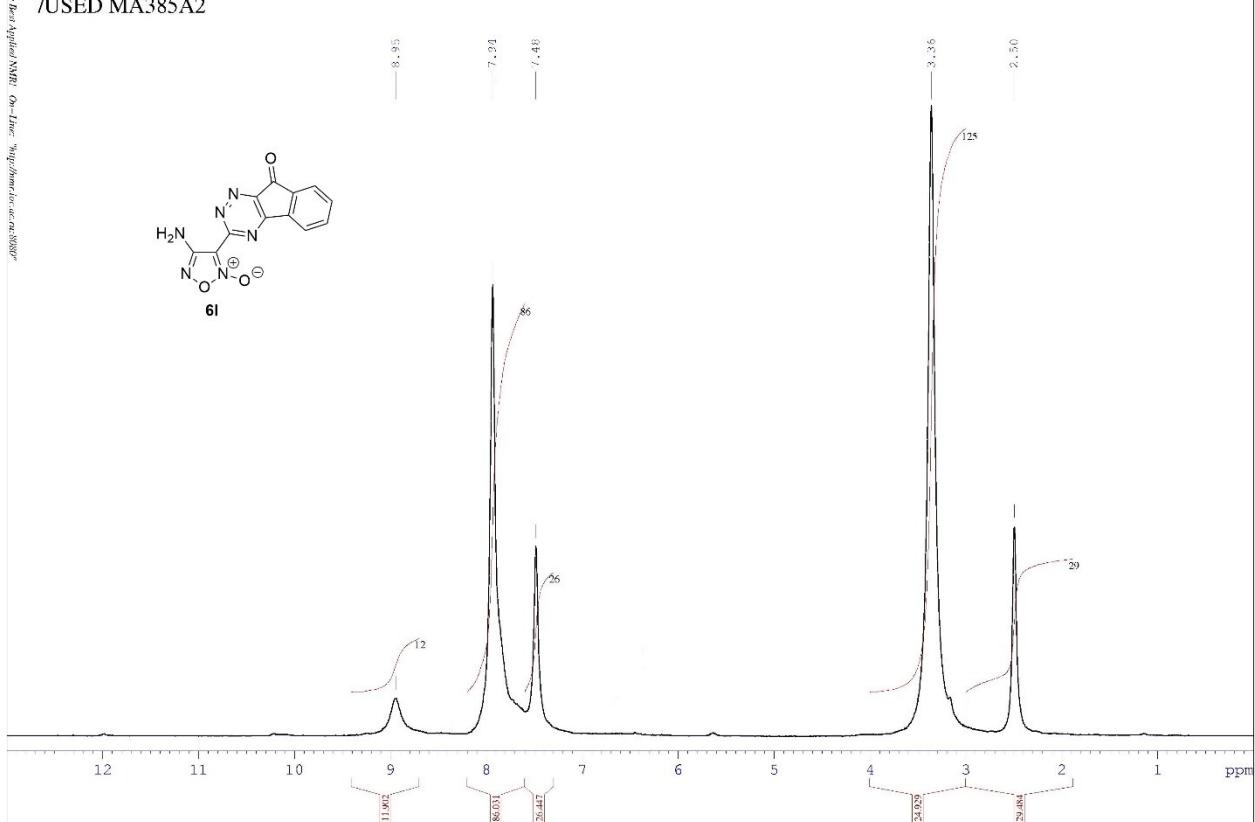
22.12.2015



¹H NMR (300 MHz, DMSO-d₆) of **6k**

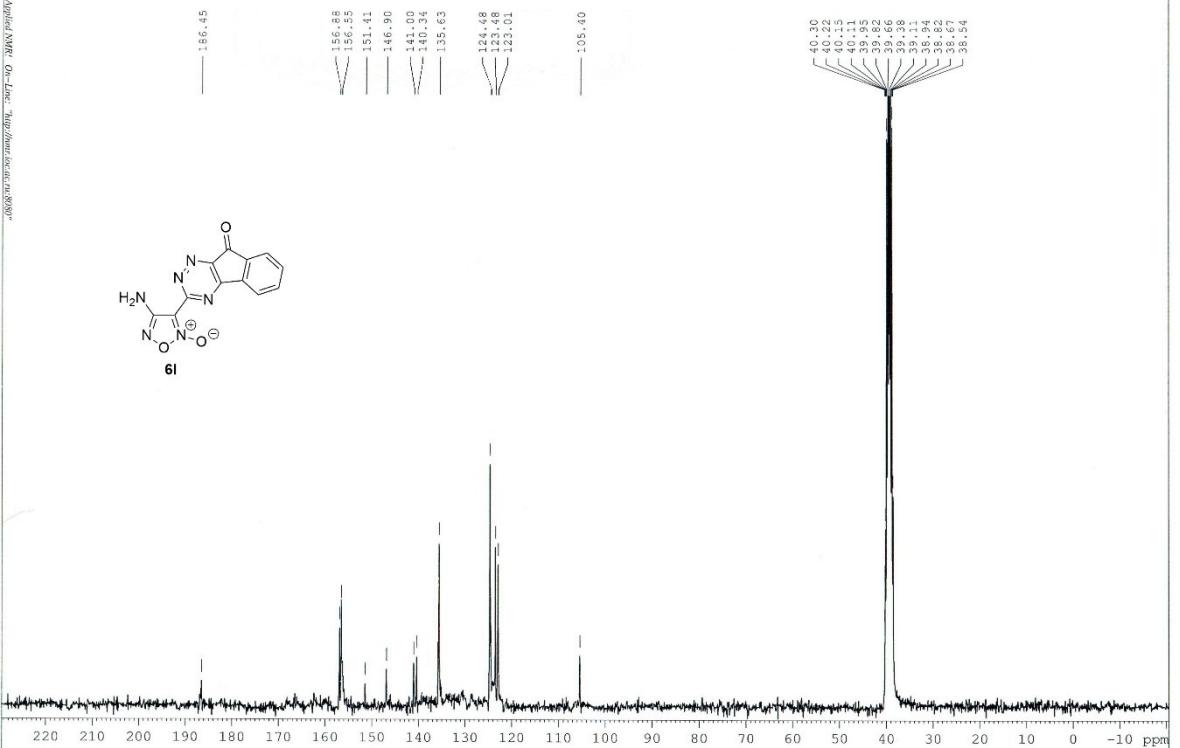


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=16K SW=7500 O1=2200 PW=9.0 AQ=1.082 RD=3.00 NS=1 SR=1.55 TE=299K 3 November 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED MA385A2

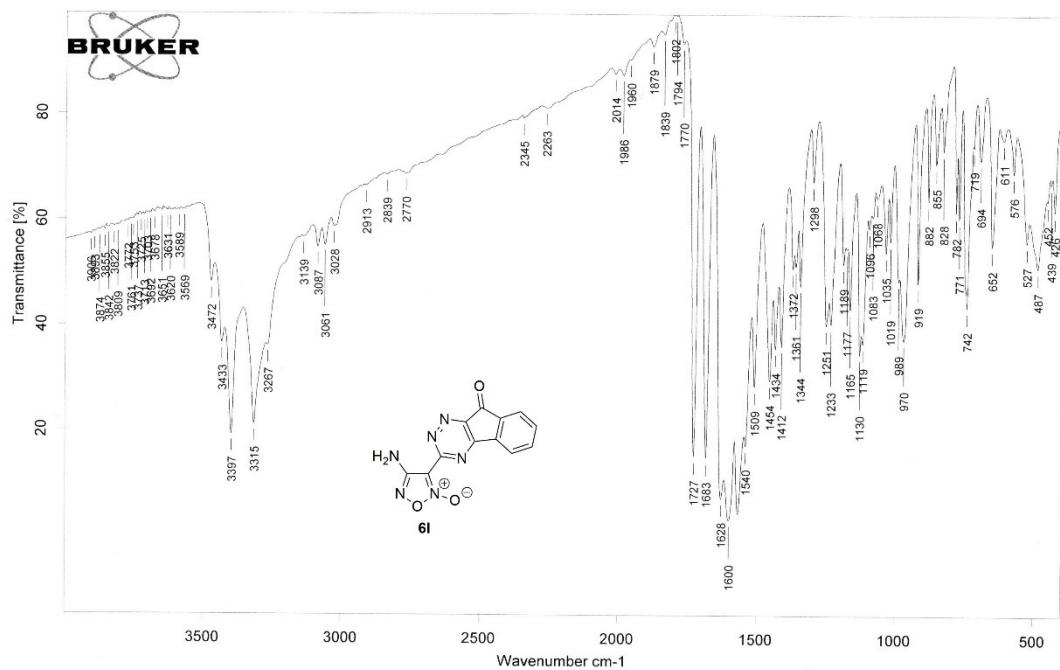


¹H NMR (300 MHz, DMSO-d₆) of **6l**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18866 O1=7920 PW=10.0 AQ=0.864 RD=2.00 NS=506 SR=38.13 TE=313K 24 November 2015 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED MA385A2



¹³C NMR (75.5 MHz, DMSO-d₆) of **6l**



D:\EDLILEO-MA385.0 ФЕРШТАТ. LEO-MA385, прессовка с KBr, 1/200.

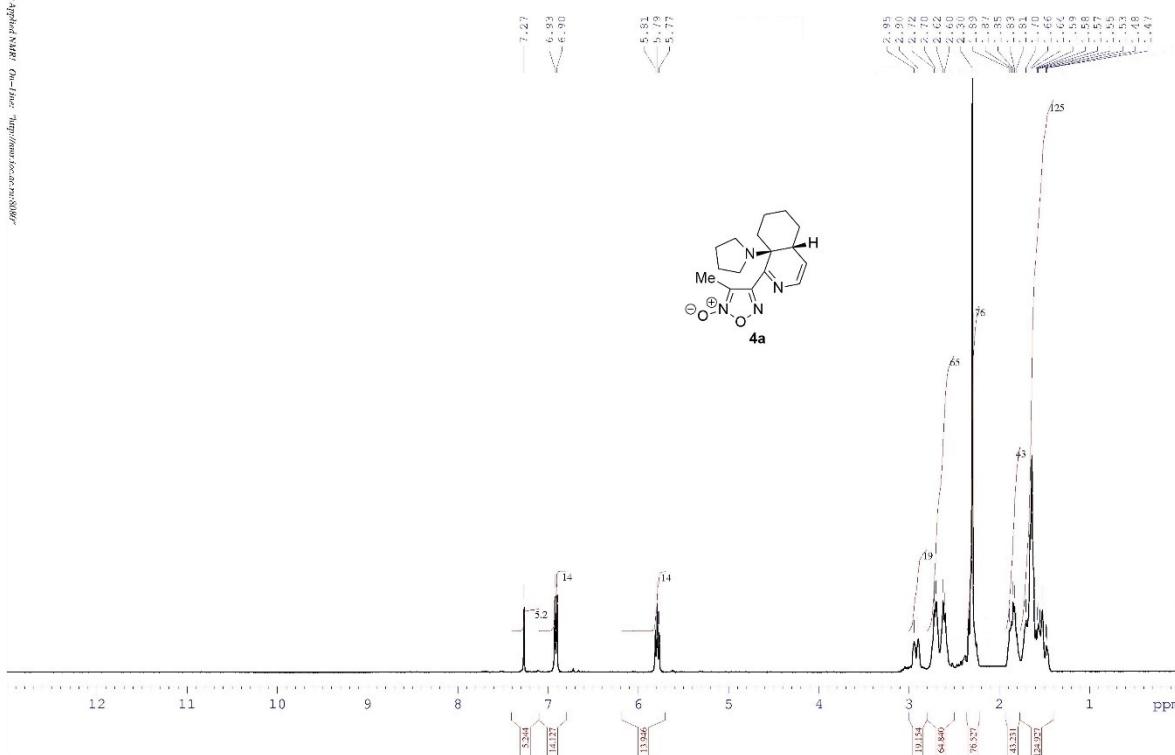
22.12.2015

Page 1/1

IR (KBr) of **6l**

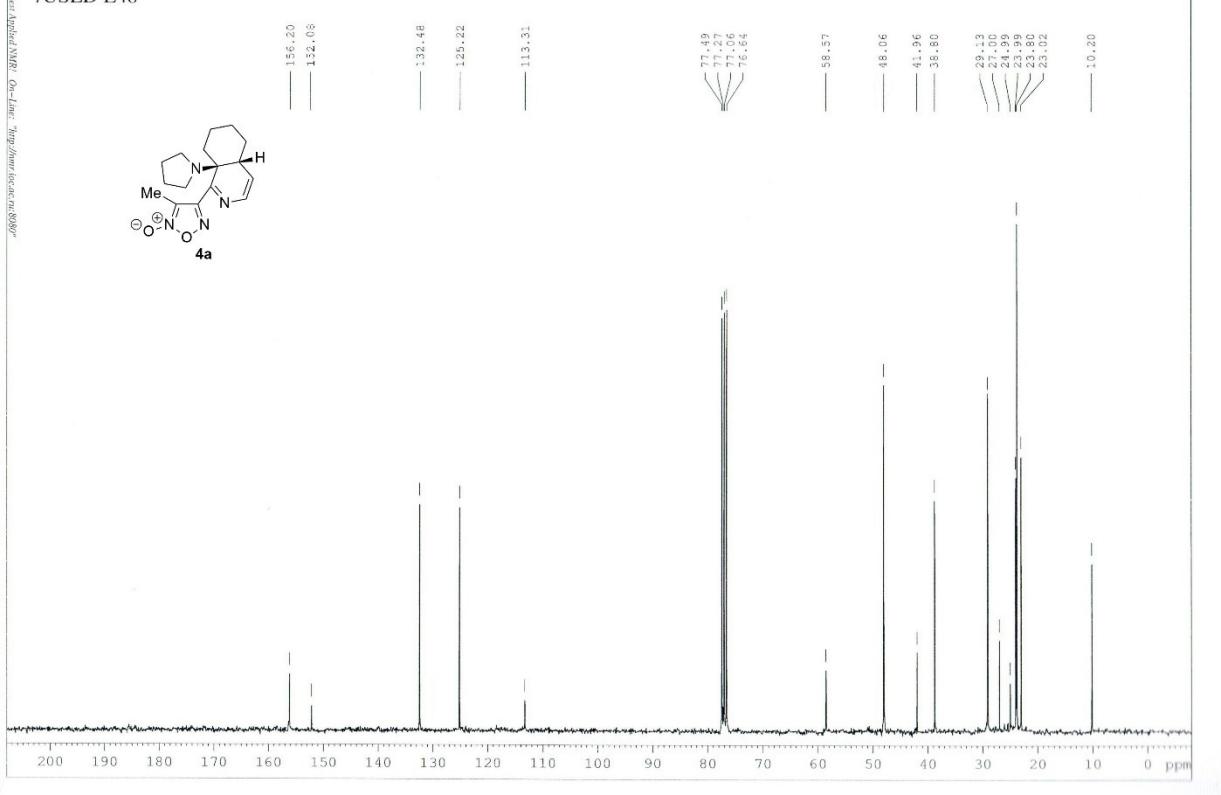
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM360 SF=300.13 MHz {1H}; ST=16K SW=7500(O)=240; FW=9.0 A Q=1.083 RD=3.01 NS=1 SR=4.15 TF=298K 12 November 2015 Opr: Strudikova M.I.; Solv: CDCl3;

/USED L48



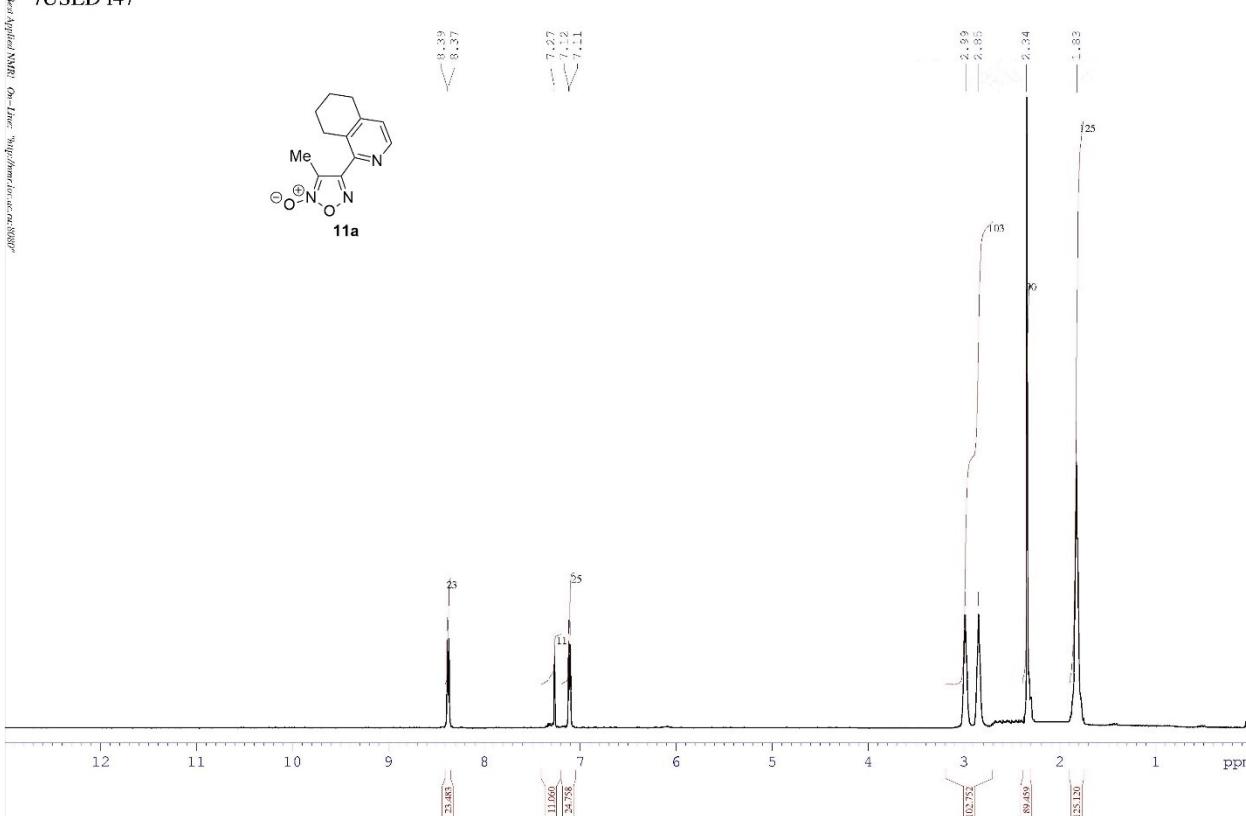
¹H NMR (300 MHz, CDCl₃) of **4a**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=2.00 NS=239 SR=—0.61 TE=298K 12 November 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED L48

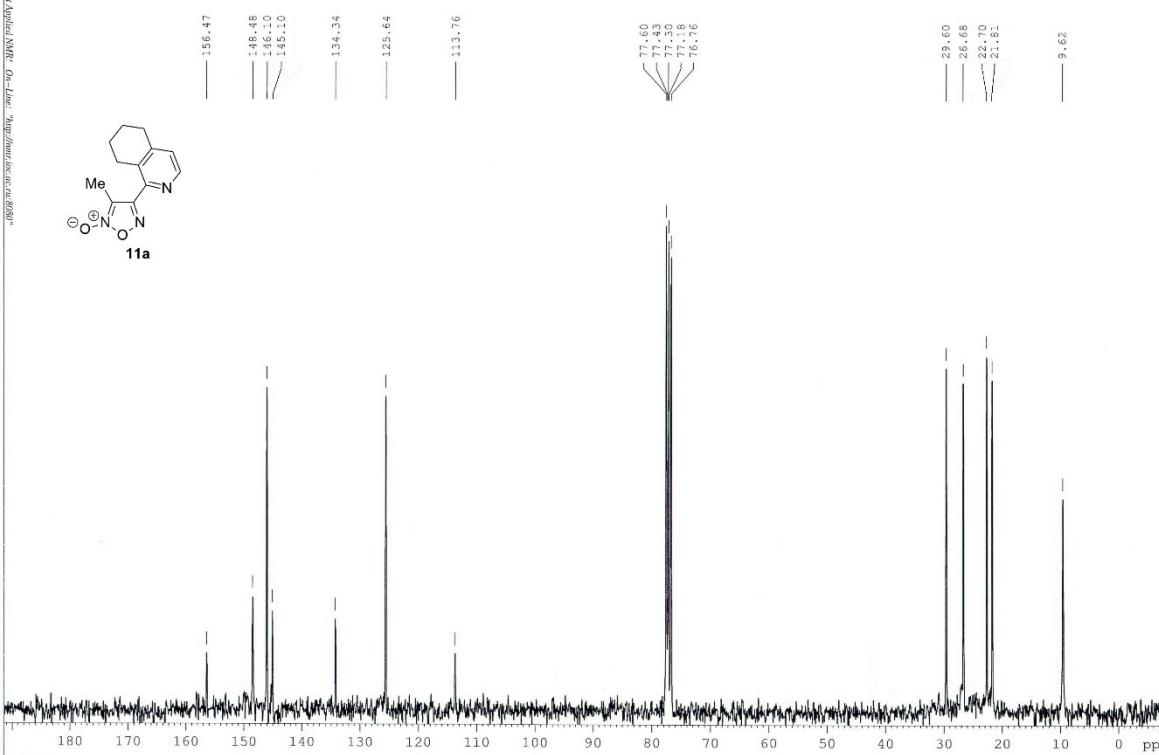


¹³C NMR (75.5 MHz, CDCl₃) of **4a**

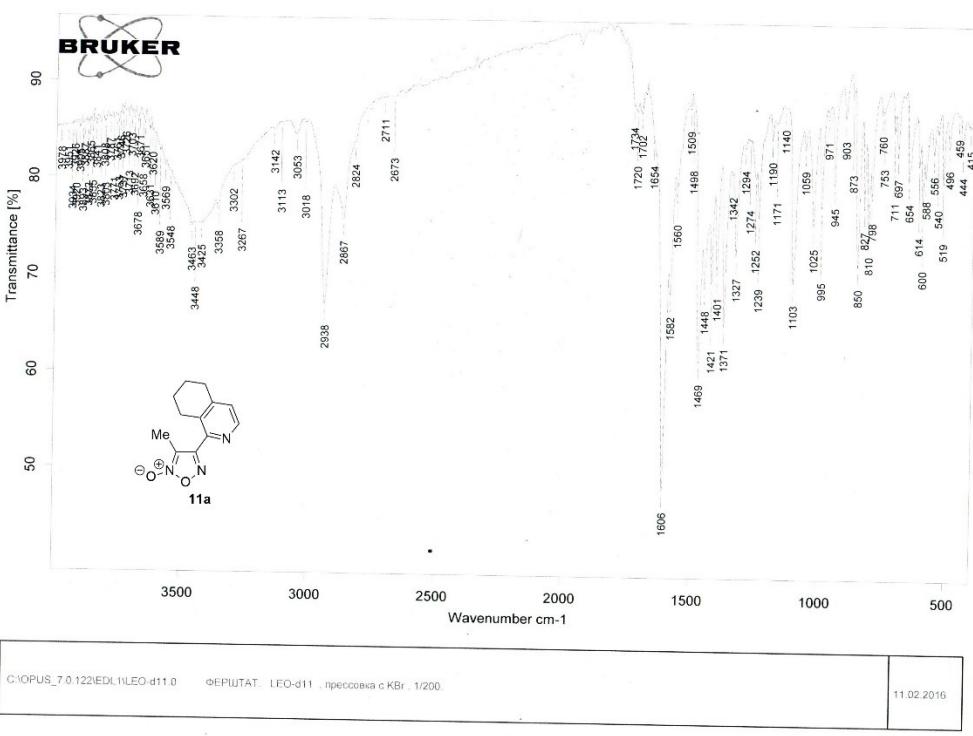
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=3.00 NS=1 SR=4.15 TE=298K 14 November 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 147



¹H NMR (300 MHz, CDCl₃) of **11a**

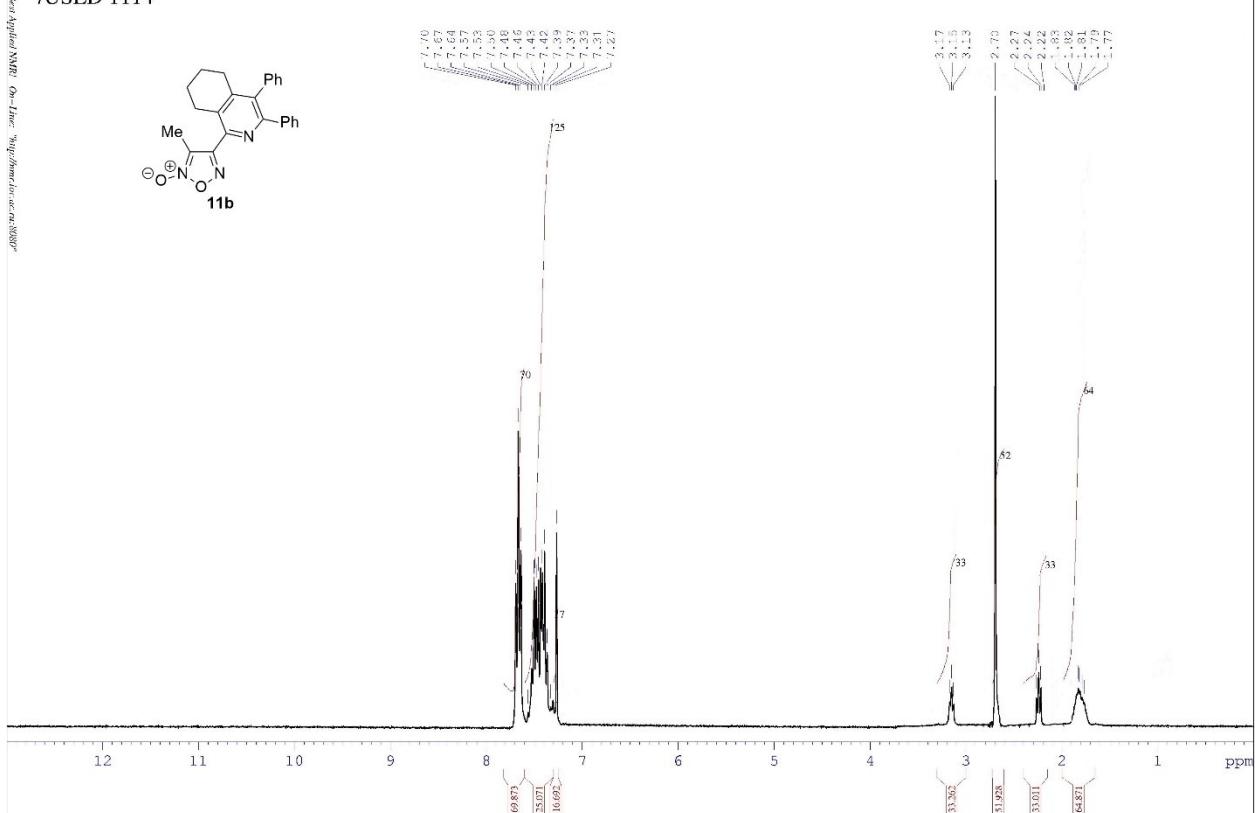


¹³C NMR (75.5 MHz, CDCl₃) of **11a**

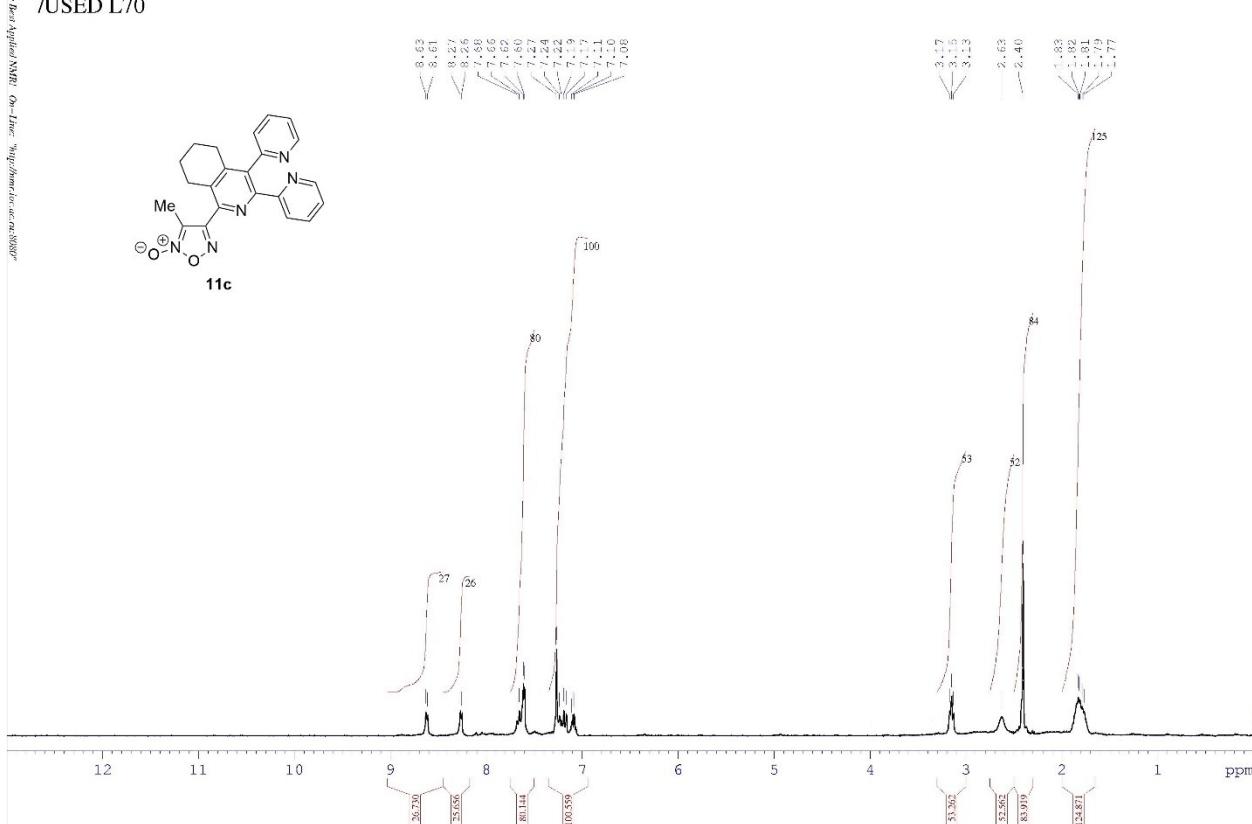


IR (KBr) of **11a**

/USED 1114

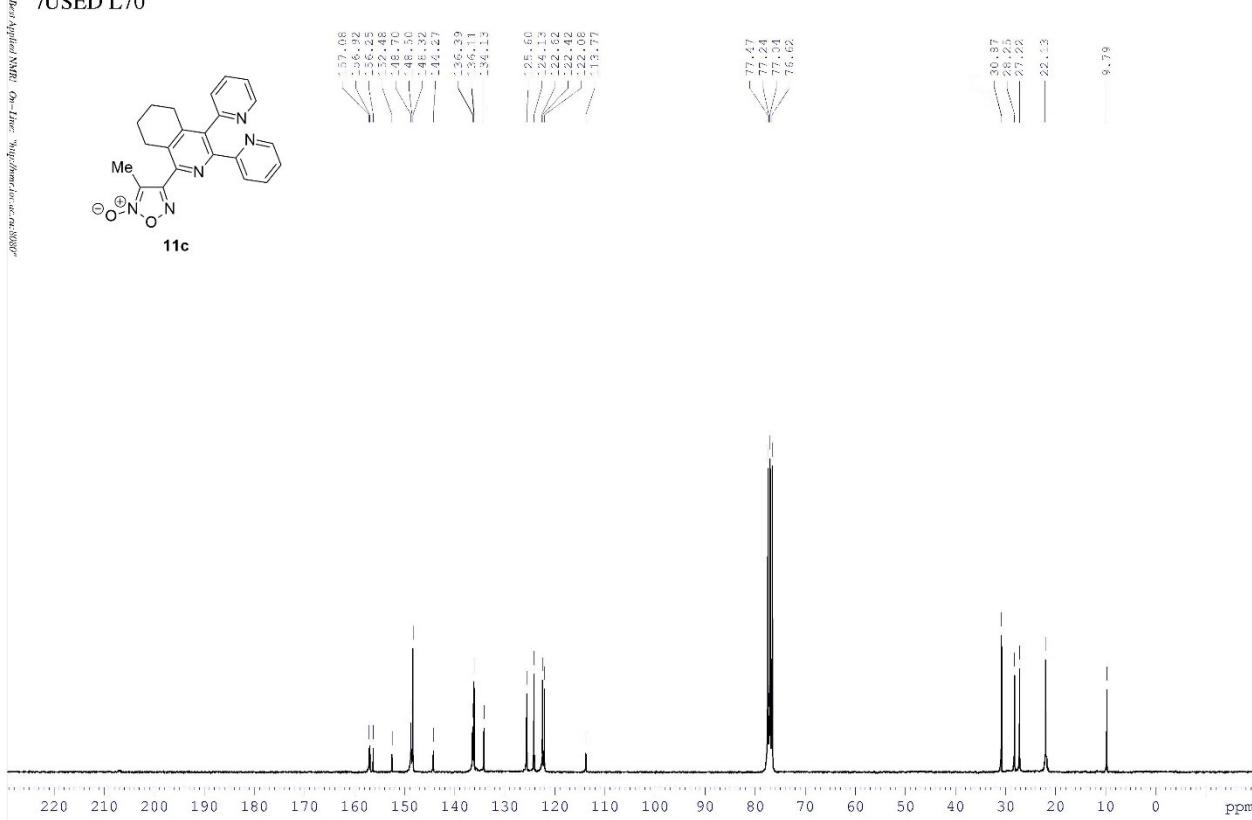


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 NS=1 SR=4.16 TE=298K 9 December 2015 Opr: Struchkova M.L.; Solv: CDCl₃; /USED L70



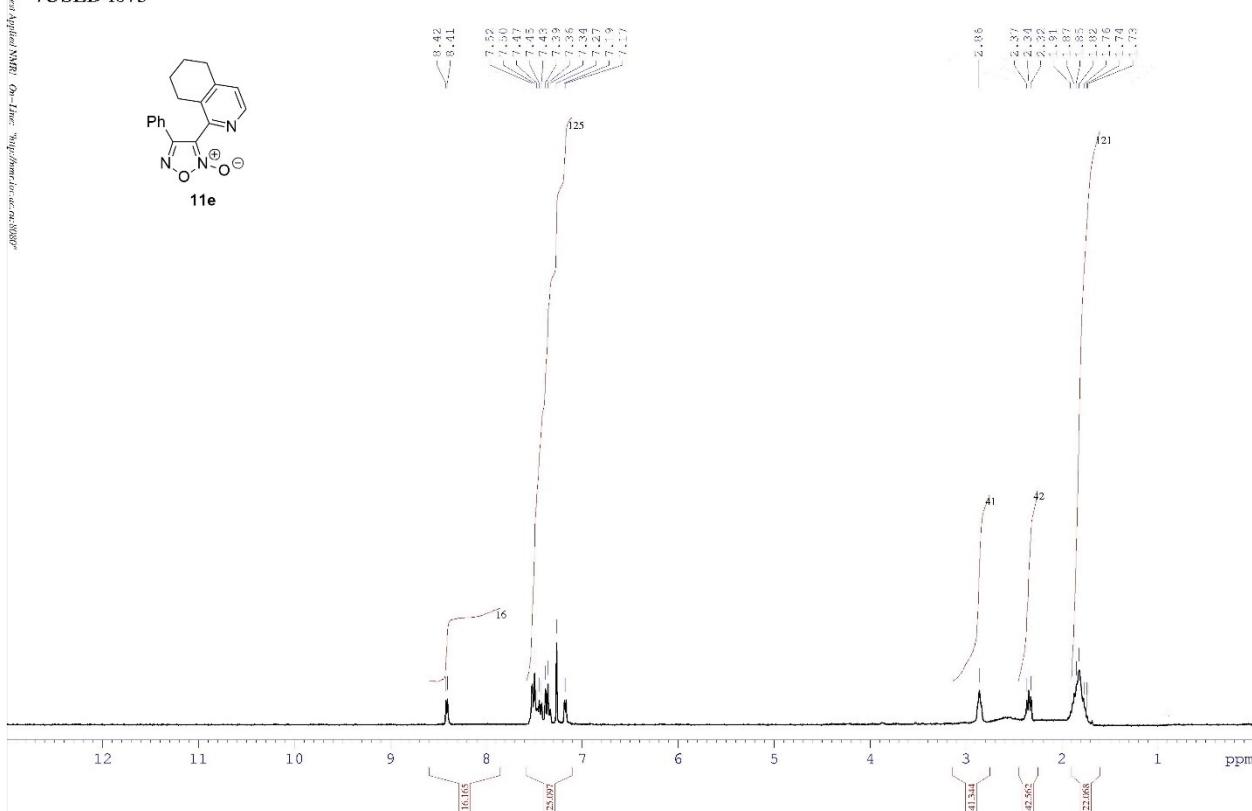
¹H NMR (300 MHz, CDCl₃) of **11c**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=2.00 NS=18073 SR=-0.61 TE=299K 15 December 2015 Opr: Struchkova M.L.; Solv: CDCl₃; /USED L70

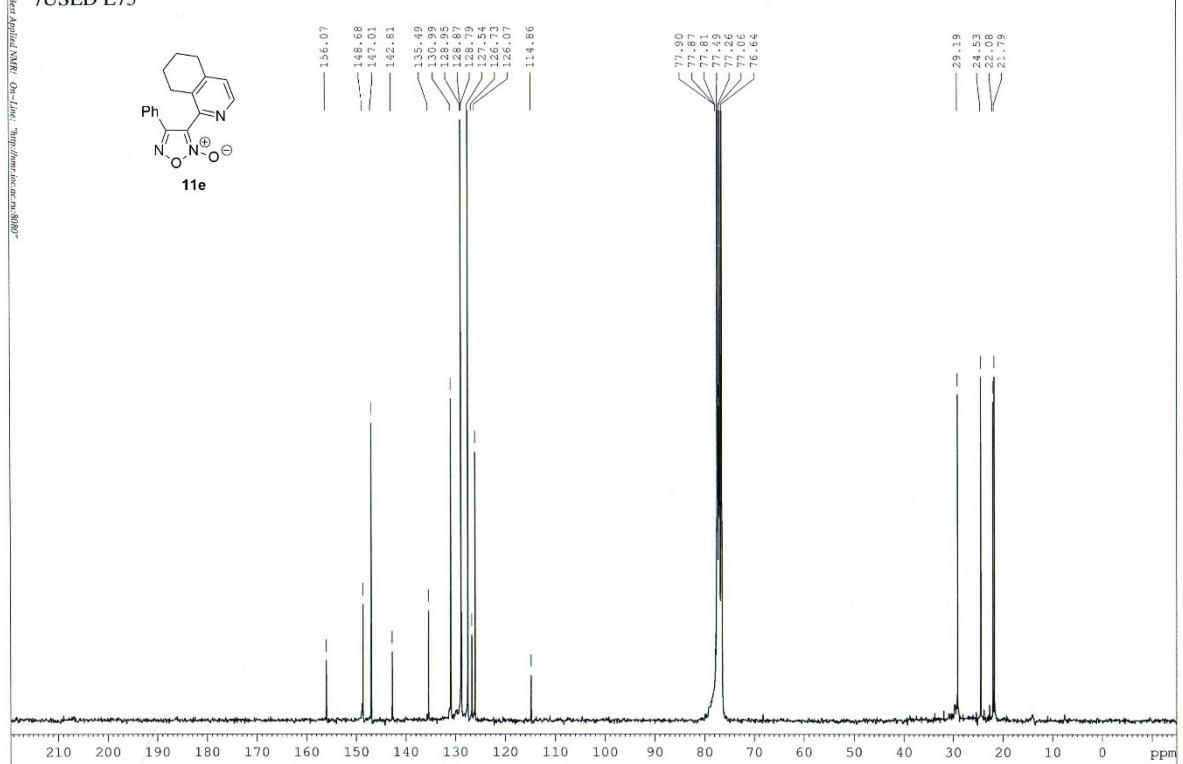


¹³C NMR (75.5 MHz, CDCl₃) of **11c**

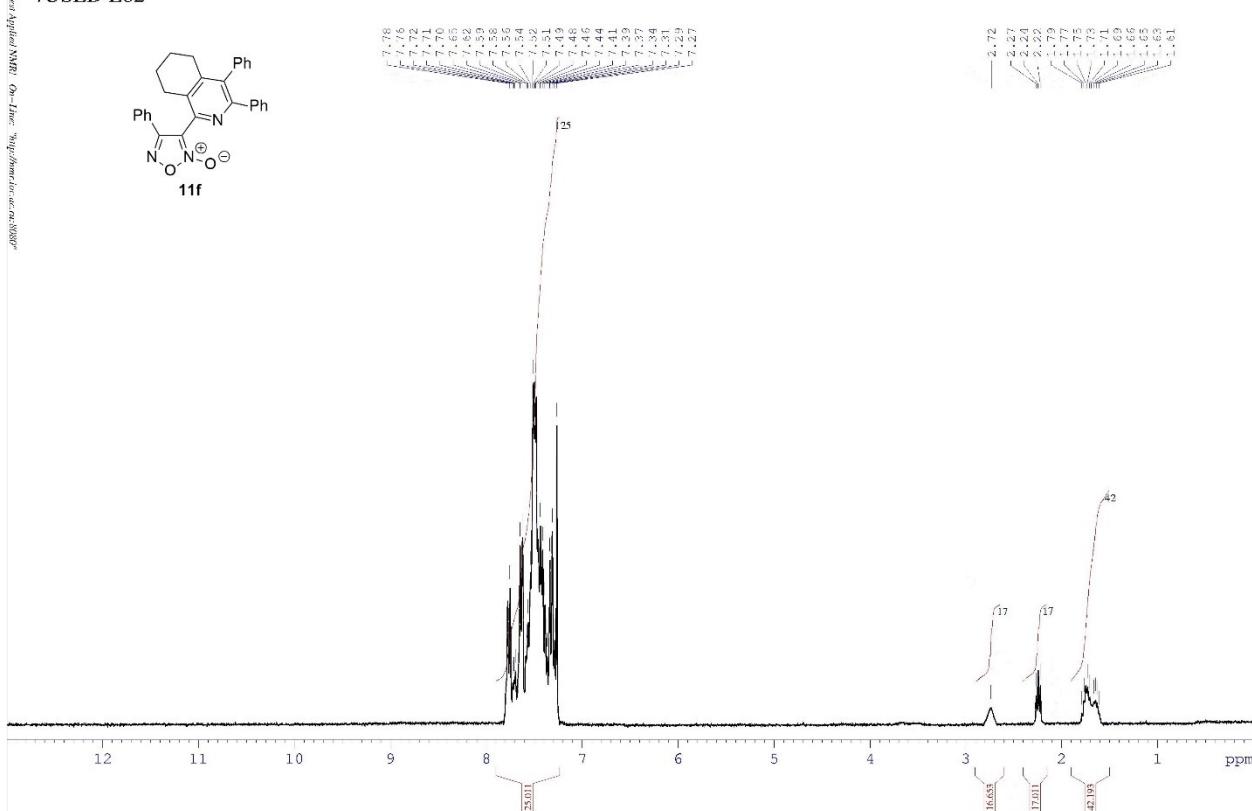
/USED 1075



/USED L75

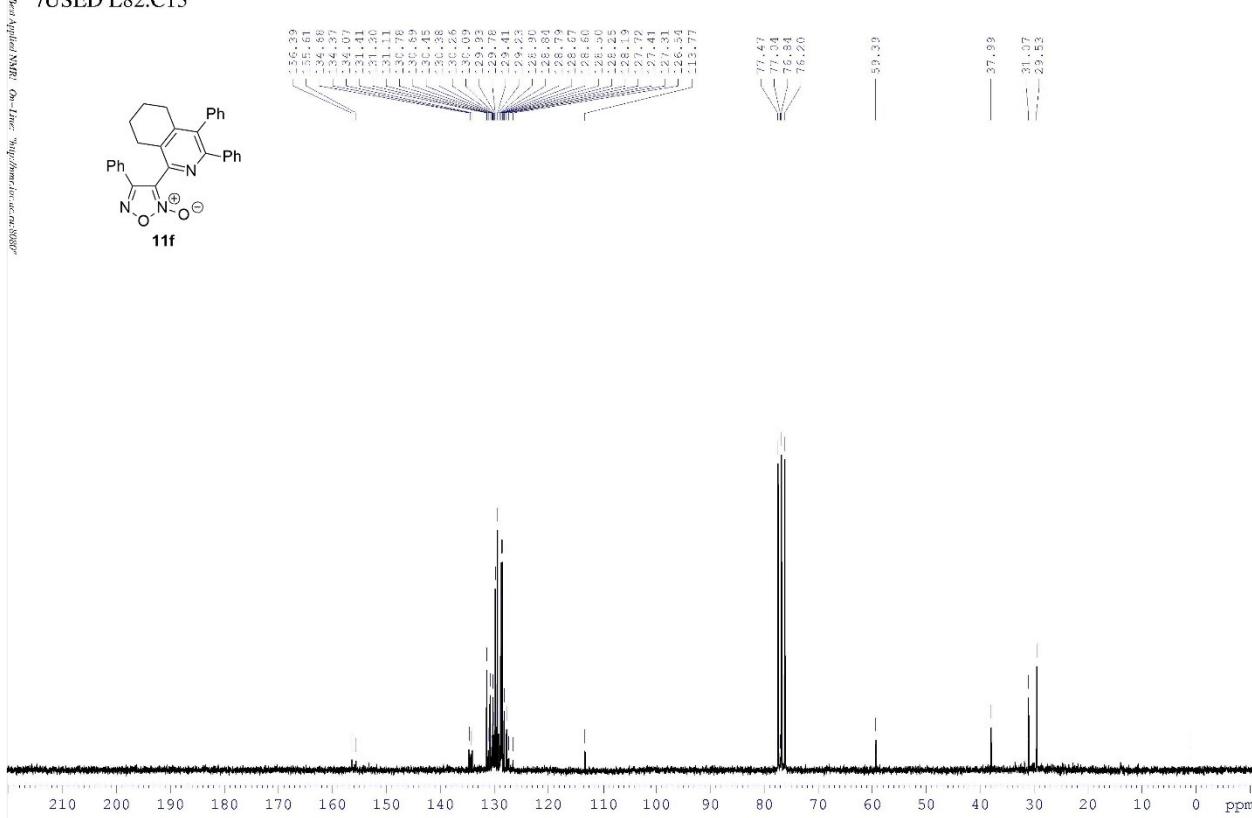


/USED L82

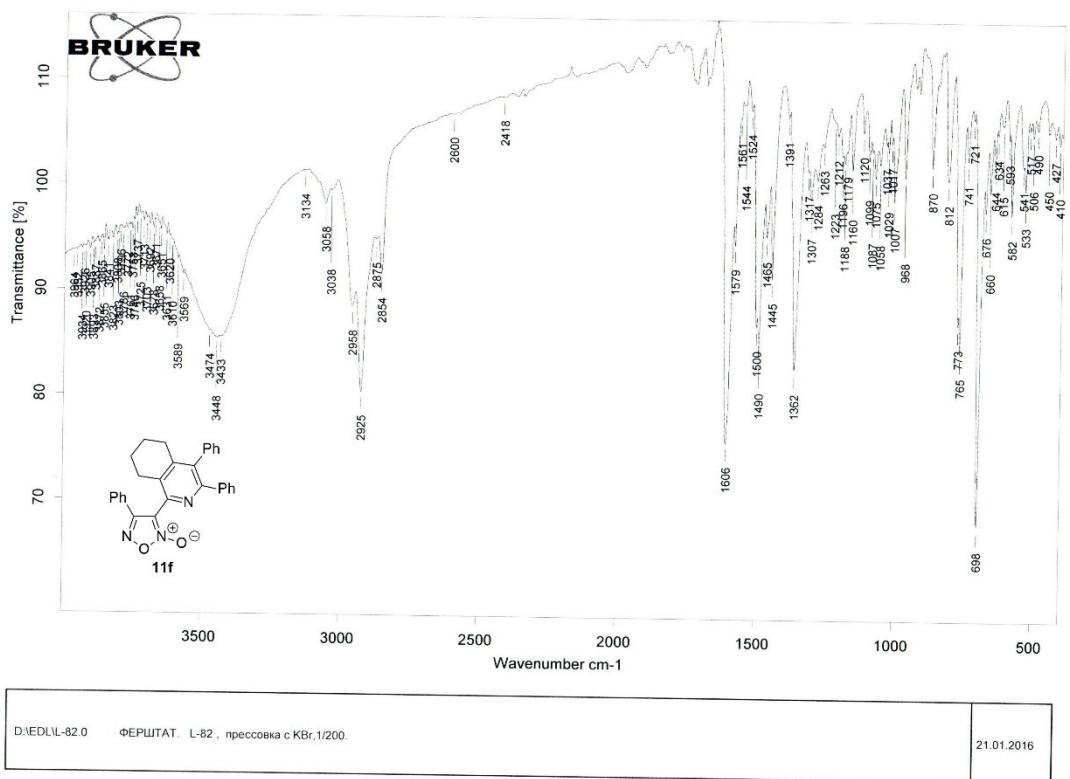


¹H NMR (300 MHz, CDCl₃) of **11f**

/USED L82.C13

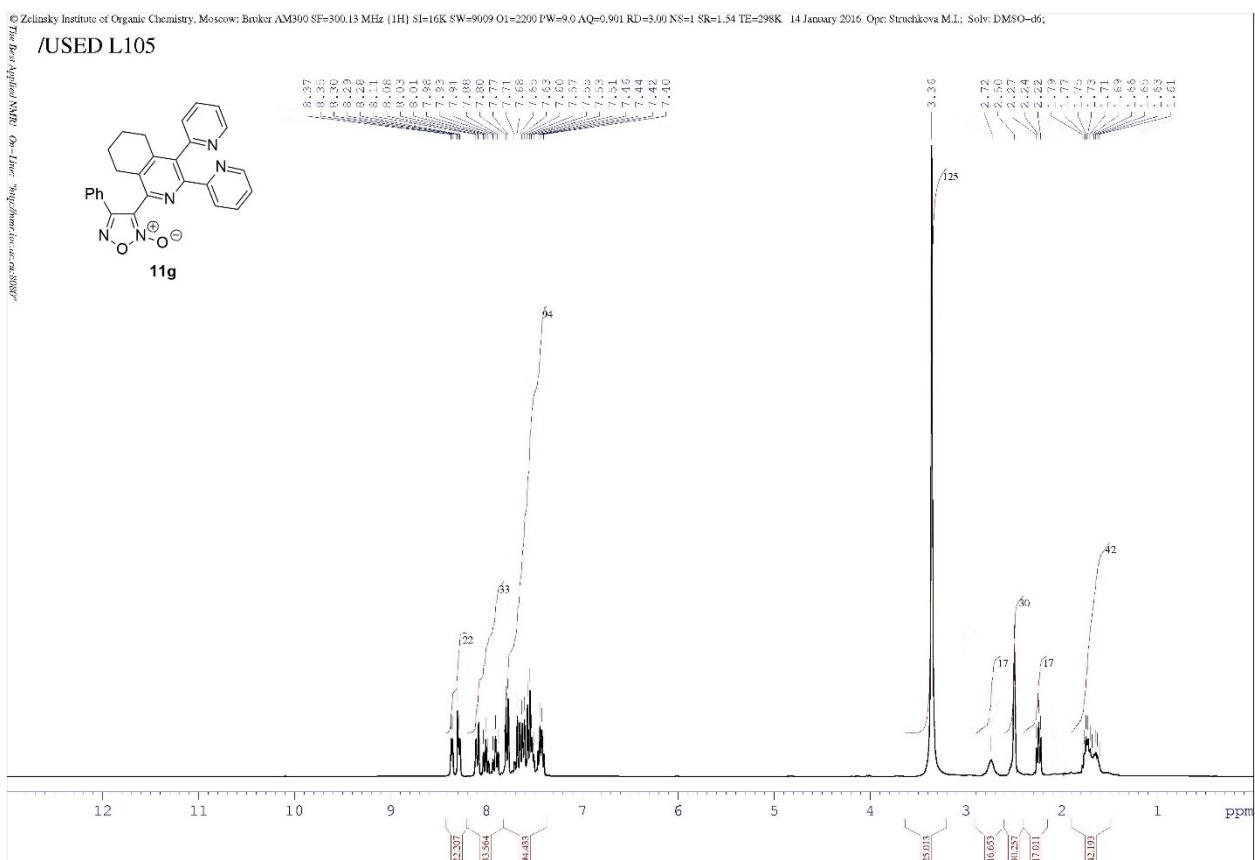


¹³C NMR (50.3 MHz, CDCl₃) of **11f**



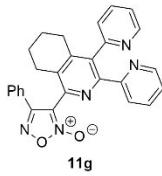
Page 1/1

IR (KBr) of **11f**

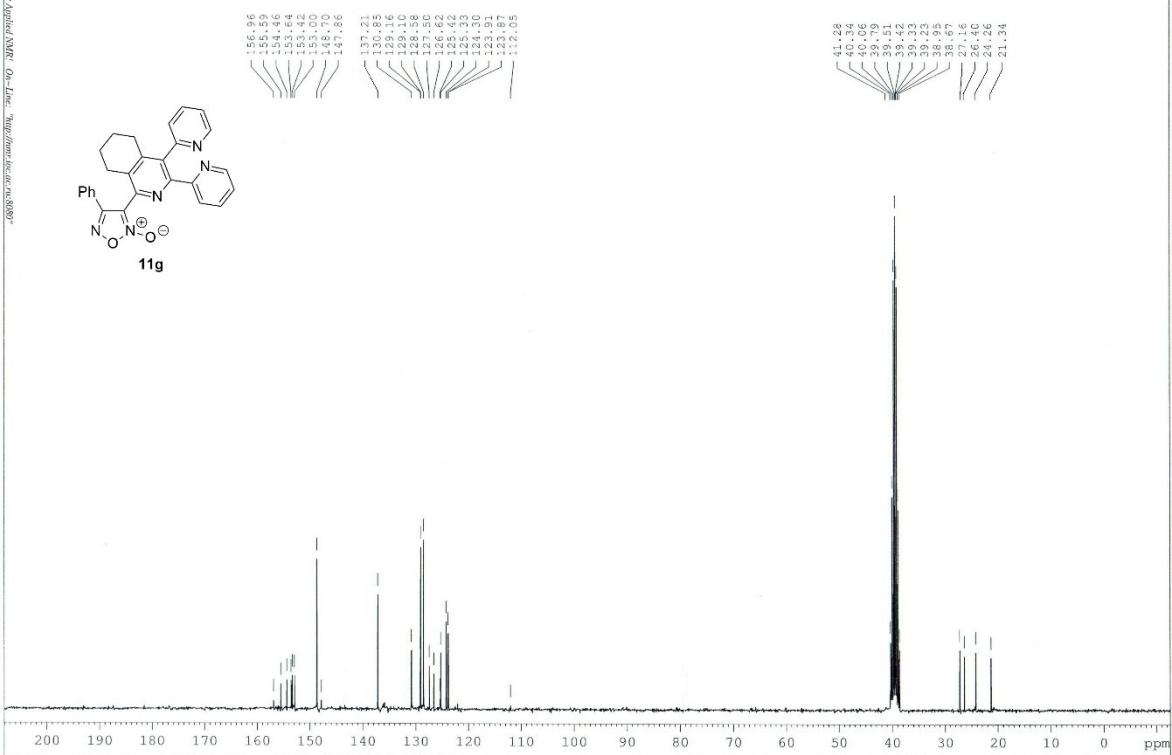


^1H NMR (300 MHz, DMSO-d₆) of **11g**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz [13C] SI=32K SW=18866 OI=7920 PW=10.0 AQ=0.864 RD=2.00 NS=128 SR=38.13 TE=300K 16 January 2016 Opr: Struchkova M.I.; Solv: DMSO-d₆; /USED L105

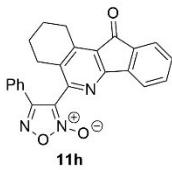


11g

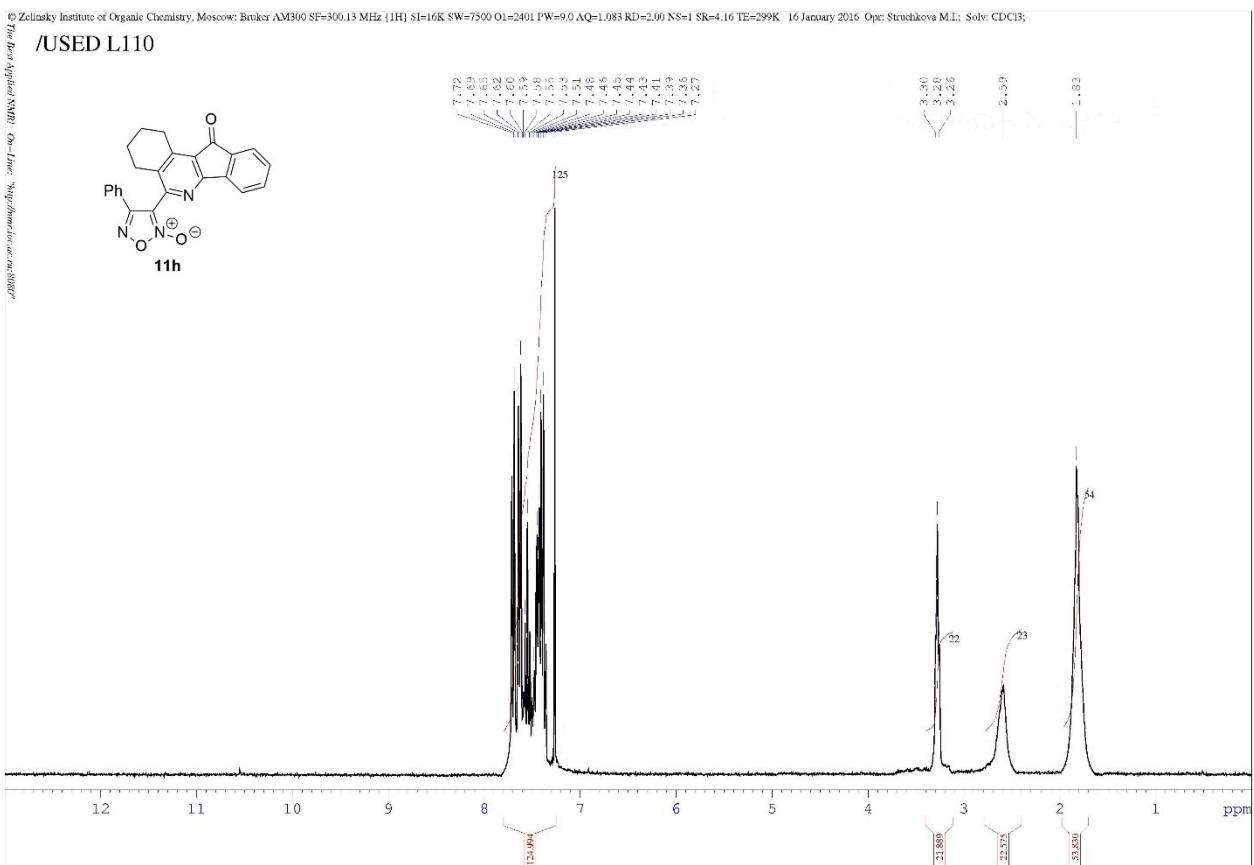


¹³C NMR (75.5 MHz, DMSO-d₆) of **11g**

© Zelinsky Institute of Organic Chemistry, Moscow; Binkov AM300 SF=300.13 MHz {1H} SI=16K SW=7500 O1=2401 PW=9.0AQ=1.083 RD=2.00 NS=1 SR=4.16 TE=299K 16 January 2016 Opt: Strukhova M.I.; Solv: CDCl₃; Prescr: Binkov

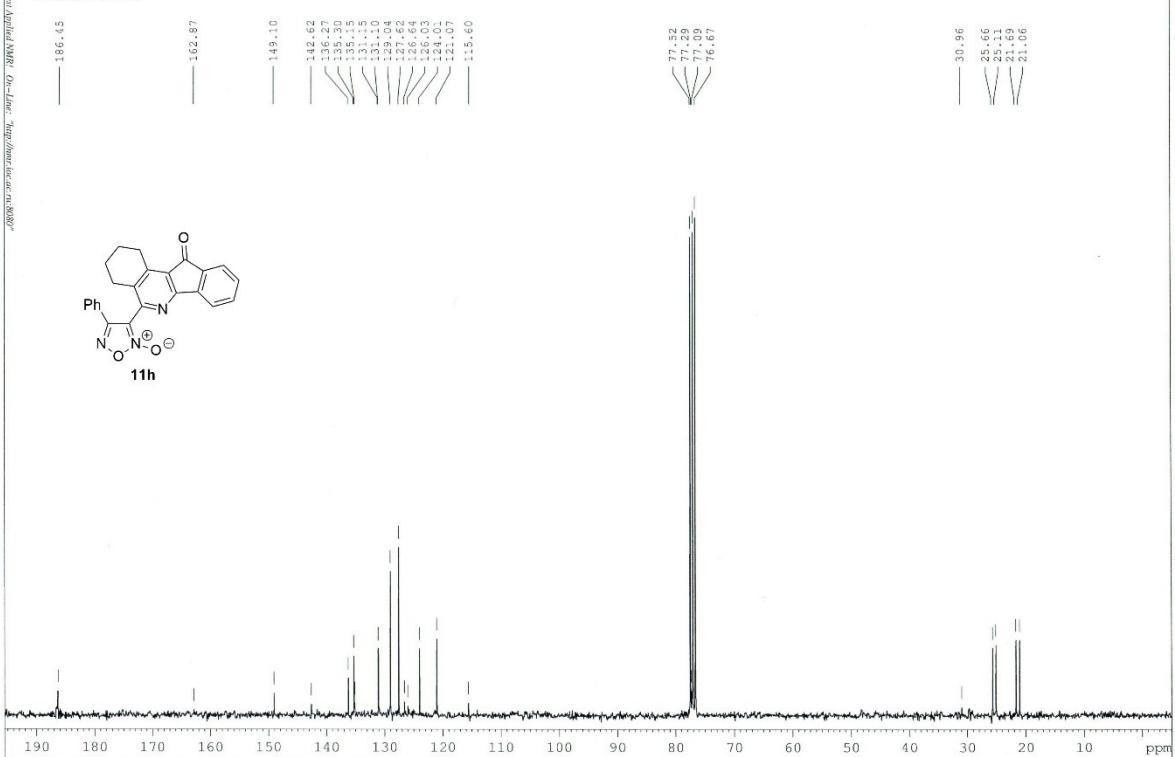


11h



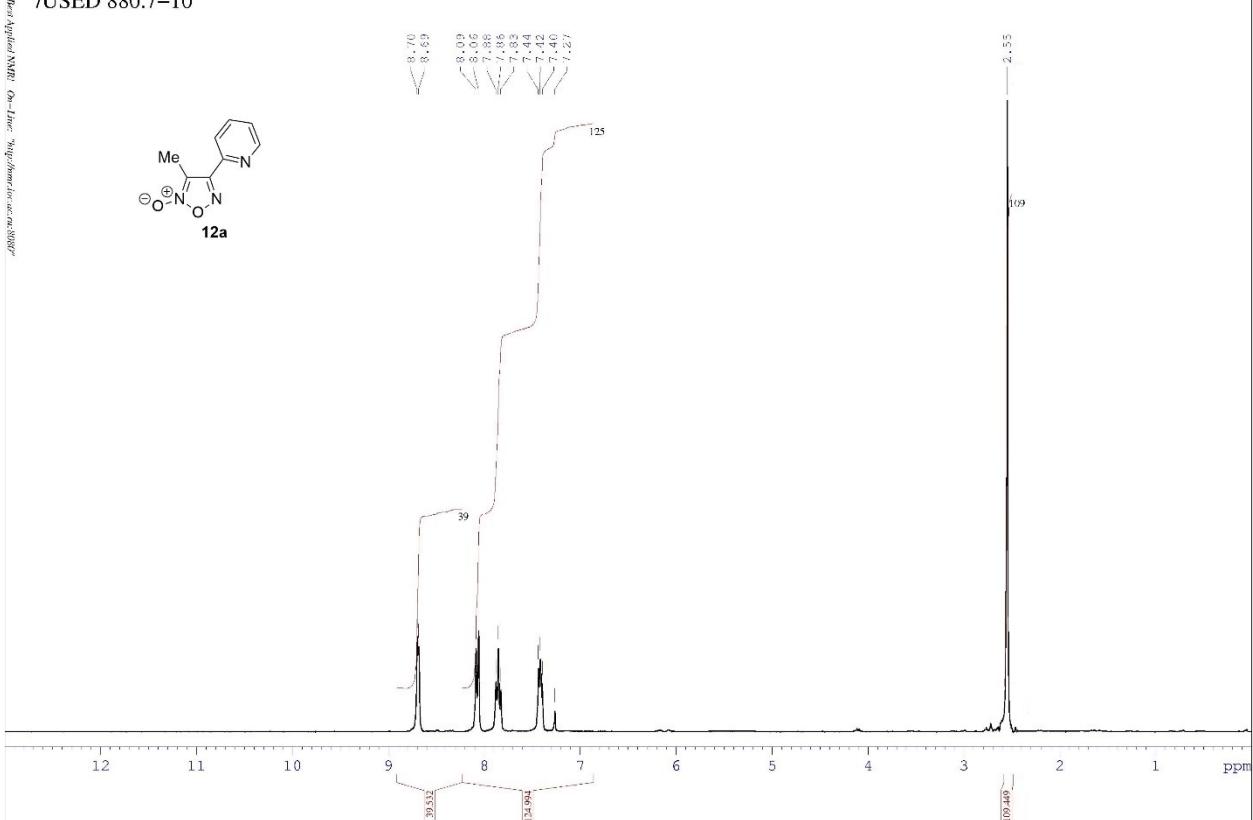
¹H NMR (300 MHz, CDCl₃) of 11h

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=2.00 NS=143 SR=5.61 TE=300K 16 January 2016 Opr: Struchkova M.I.; Solv: CDCl₃; /USED L110



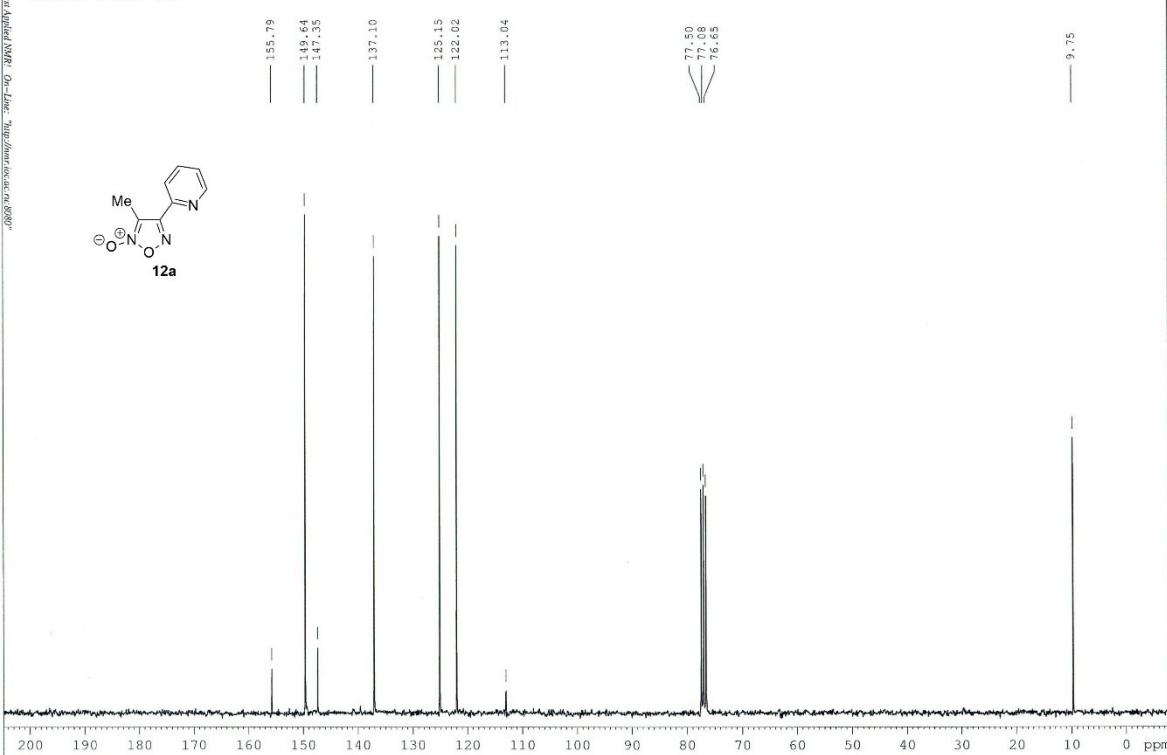
¹³C NMR (75.5 MHz, CDCl₃) of **11h**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 NS=1 SR=4.16 TE=298K 9 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 880.7-10



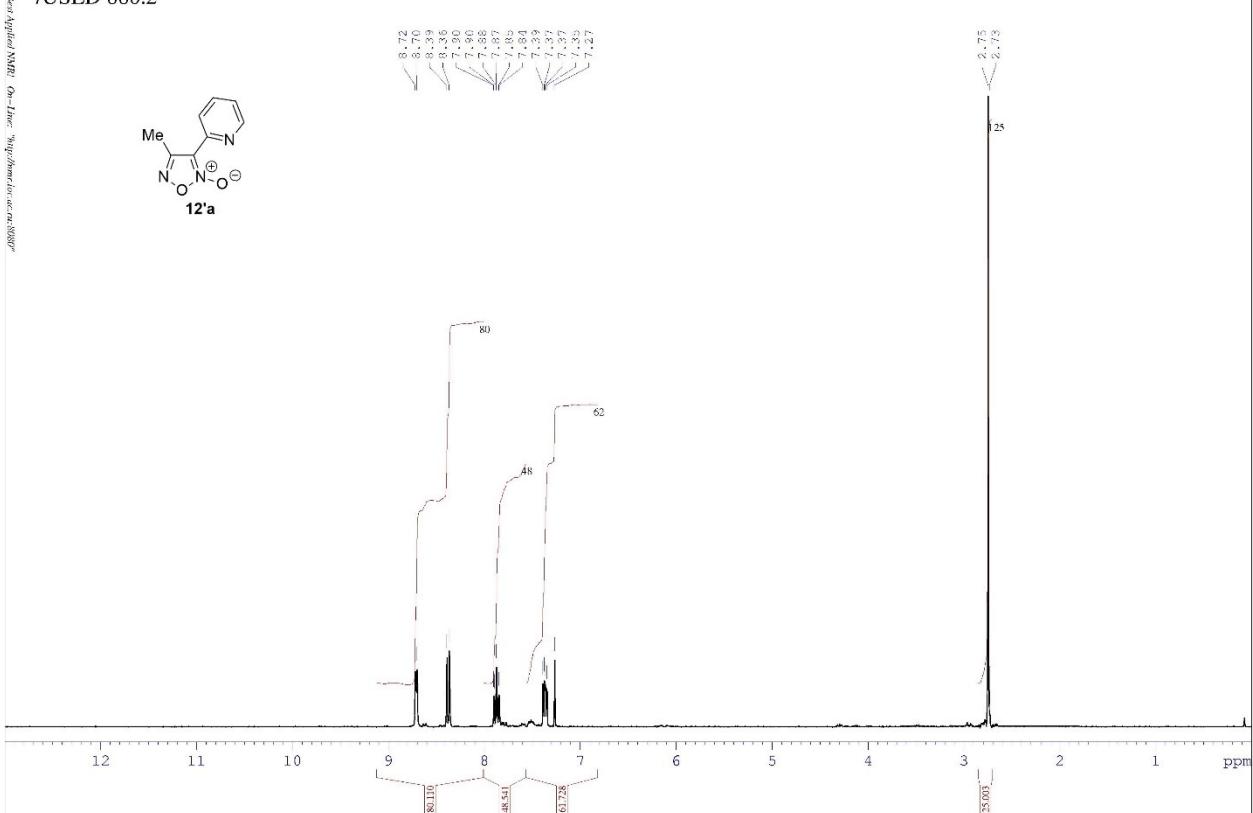
¹H NMR (300 MHz, CDCl₃) of **12a**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=1.00 NS=189 SR=-0.61 TE=299K 10 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 880.7–10



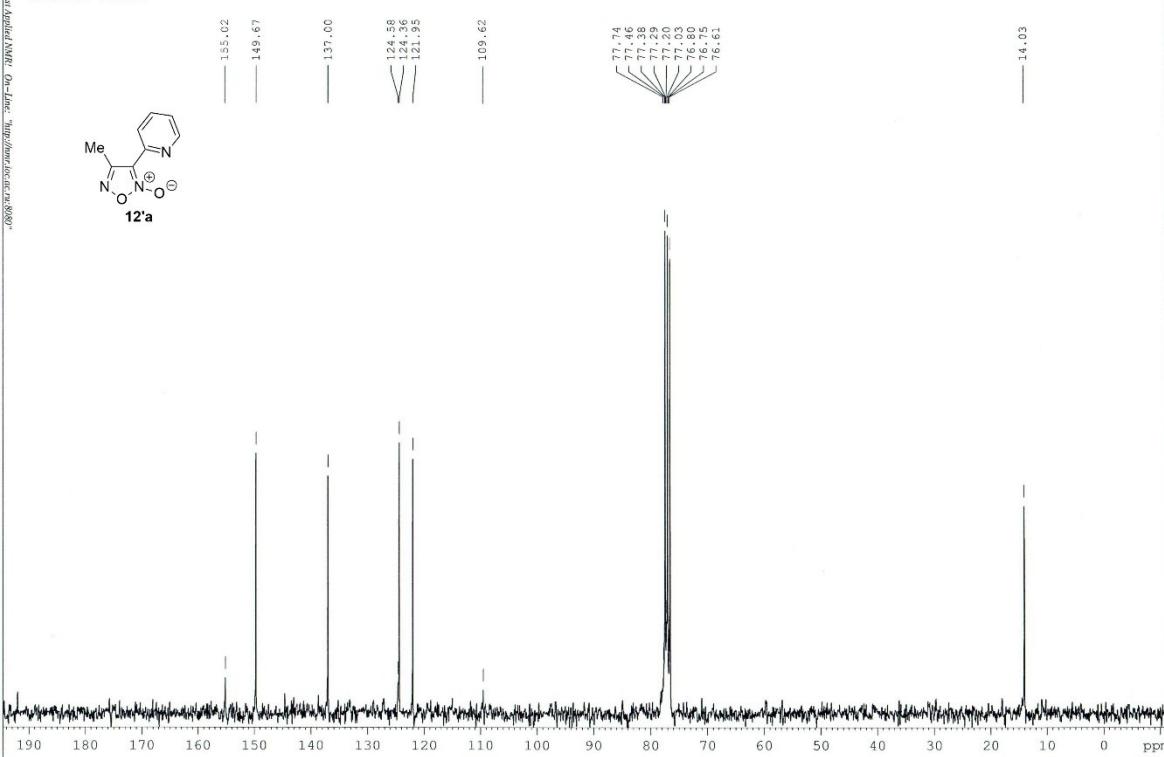
¹³C NMR (75.5 MHz, CDCl₃) of **12a**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 NS=1 SR=4.16 TE=298K 8 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 880.2

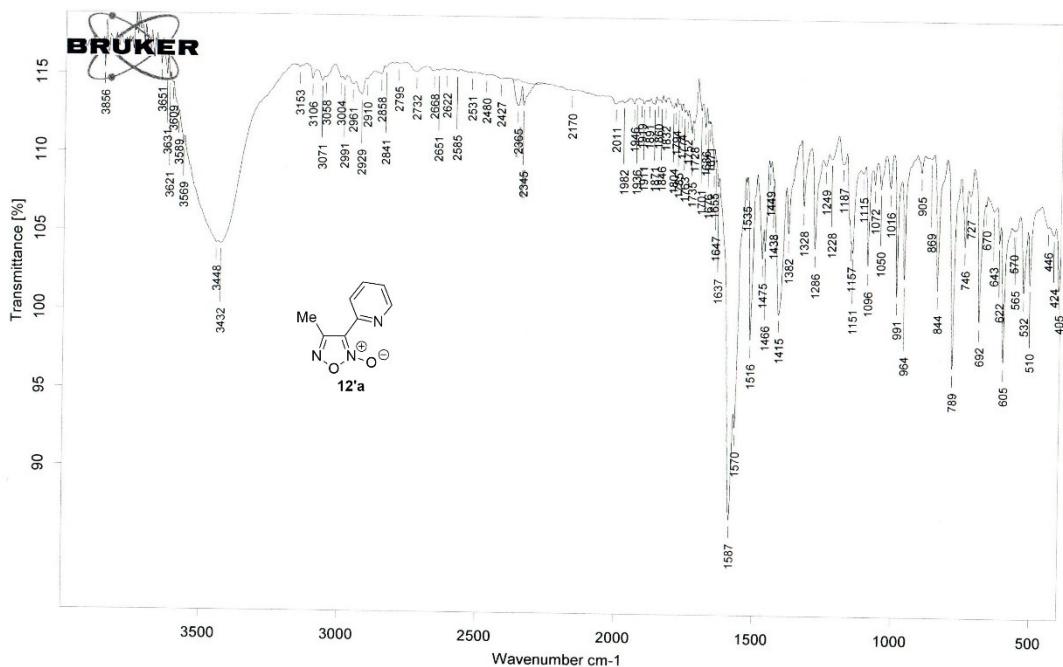


¹H NMR (300 MHz, CDCl₃) of **12'a**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=1.00 NS=303 SR=-0.61 TE=299K 10 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 880.2



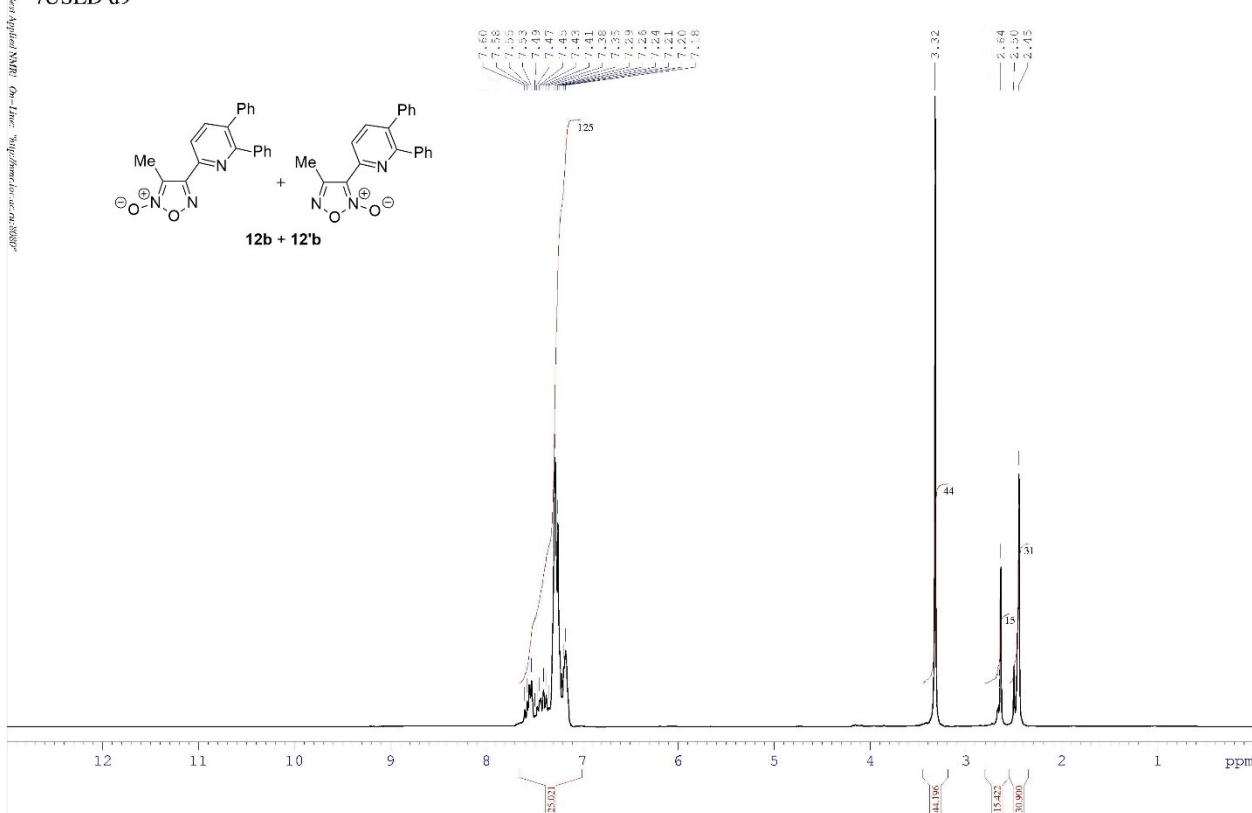
¹³C NMR (75.5 MHz, CDCl₃) of 12'a



D:\EDL\LEO-880-2.0 ФЕРШТАТ. LEO-880-2, прессовка с KBr, 1/200.

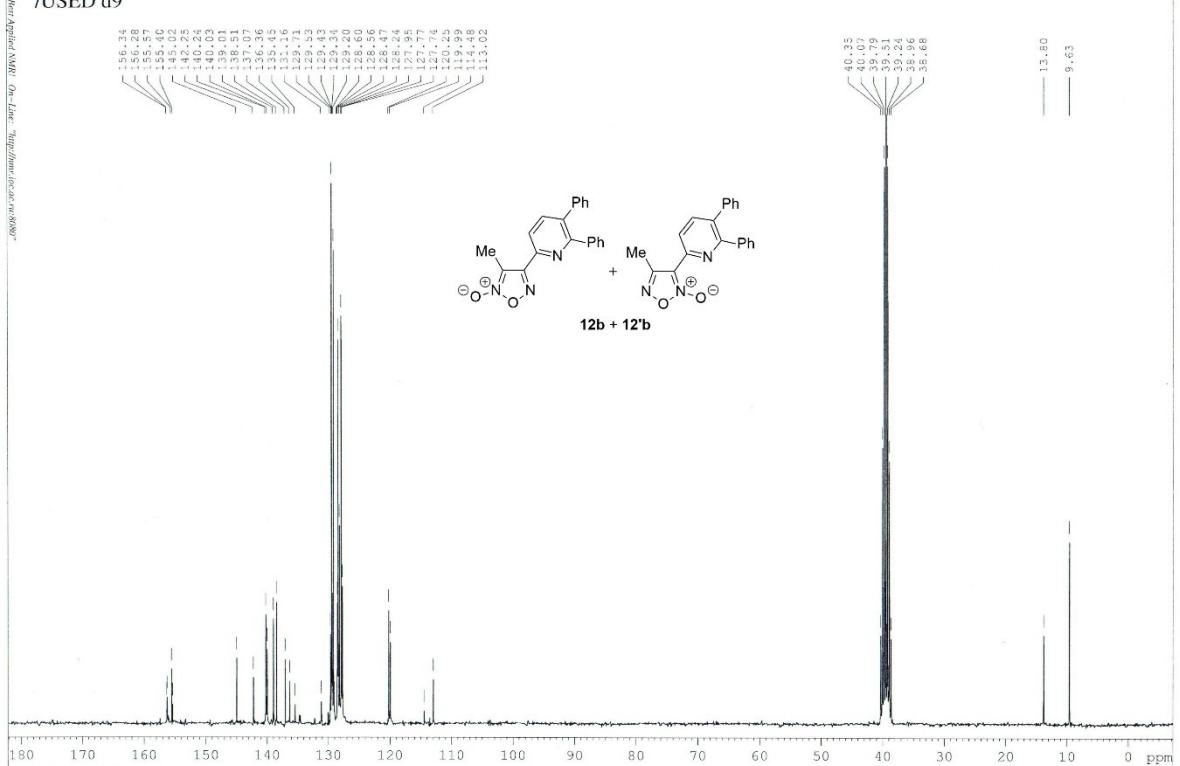
18.01.2016

/USED d9

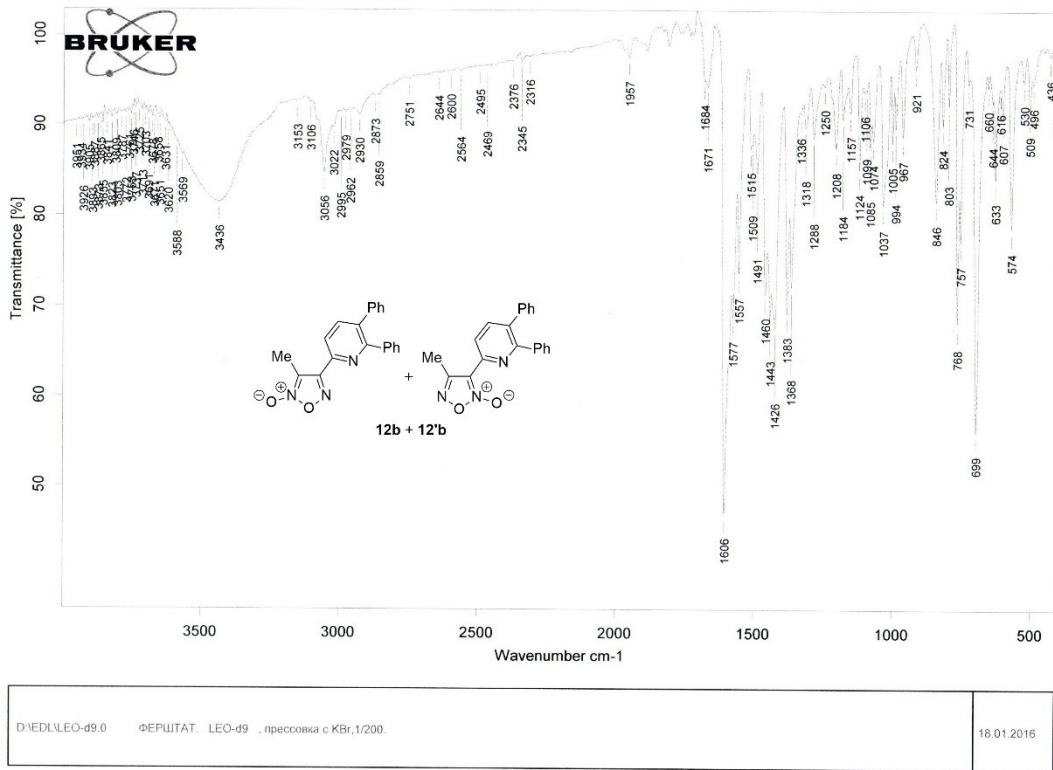


¹H NMR (300 MHz, DMSO-d₆) of a mixture **12b** + **12'b**

/USED d9

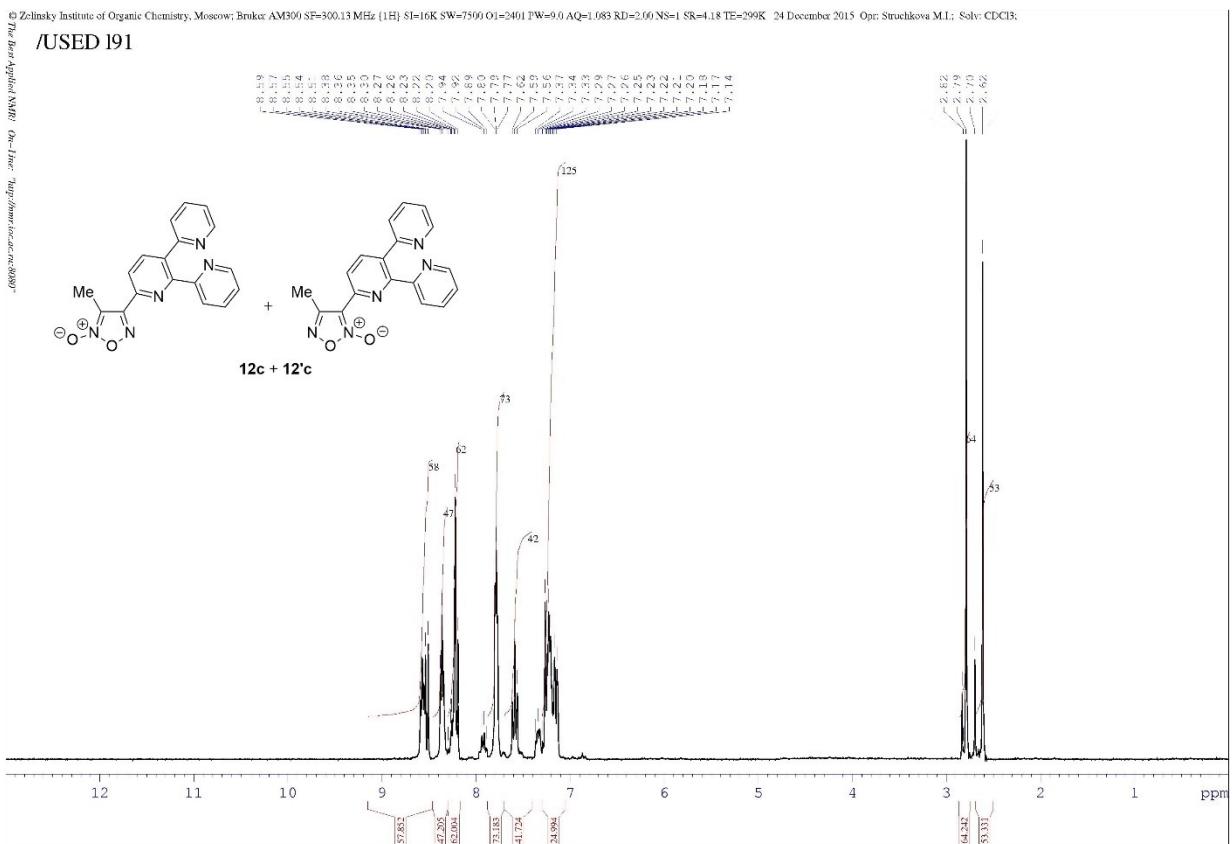


¹³C NMR (75.5 MHz, DMSO-d₆) of a mixture **12b** + **12'b**



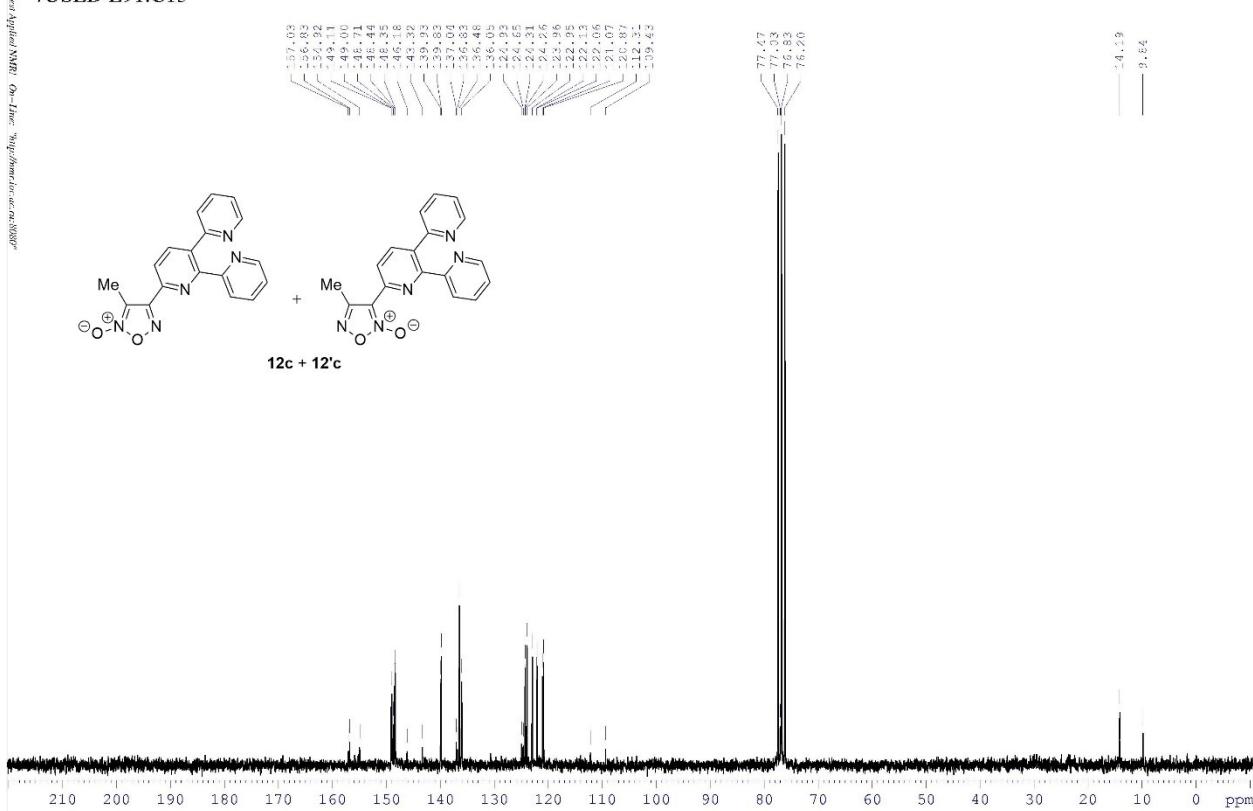
Page 1/1

IR (KBr) of a mixture **12b + 12'b**



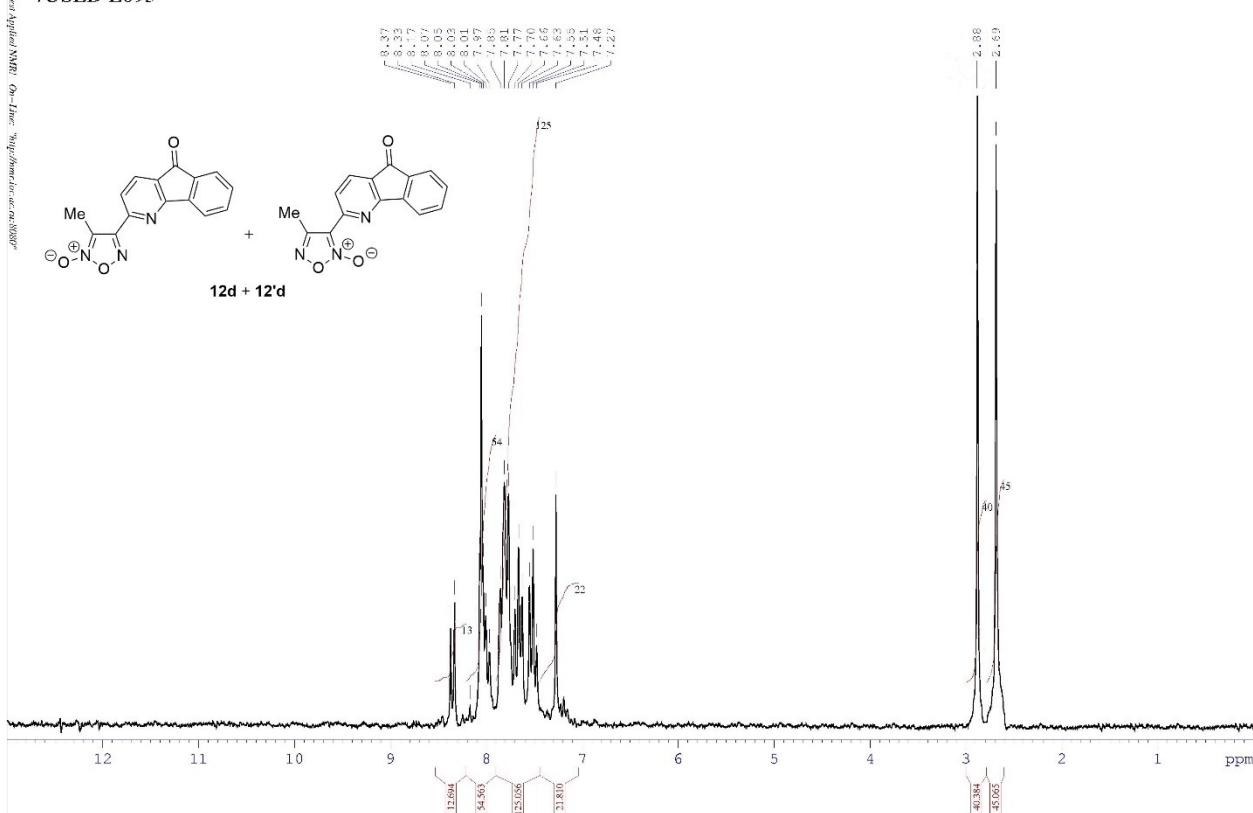
¹H NMR (300 MHz, CDCl₃) of a mixture **12c + 12'c**

/USED L91.C13



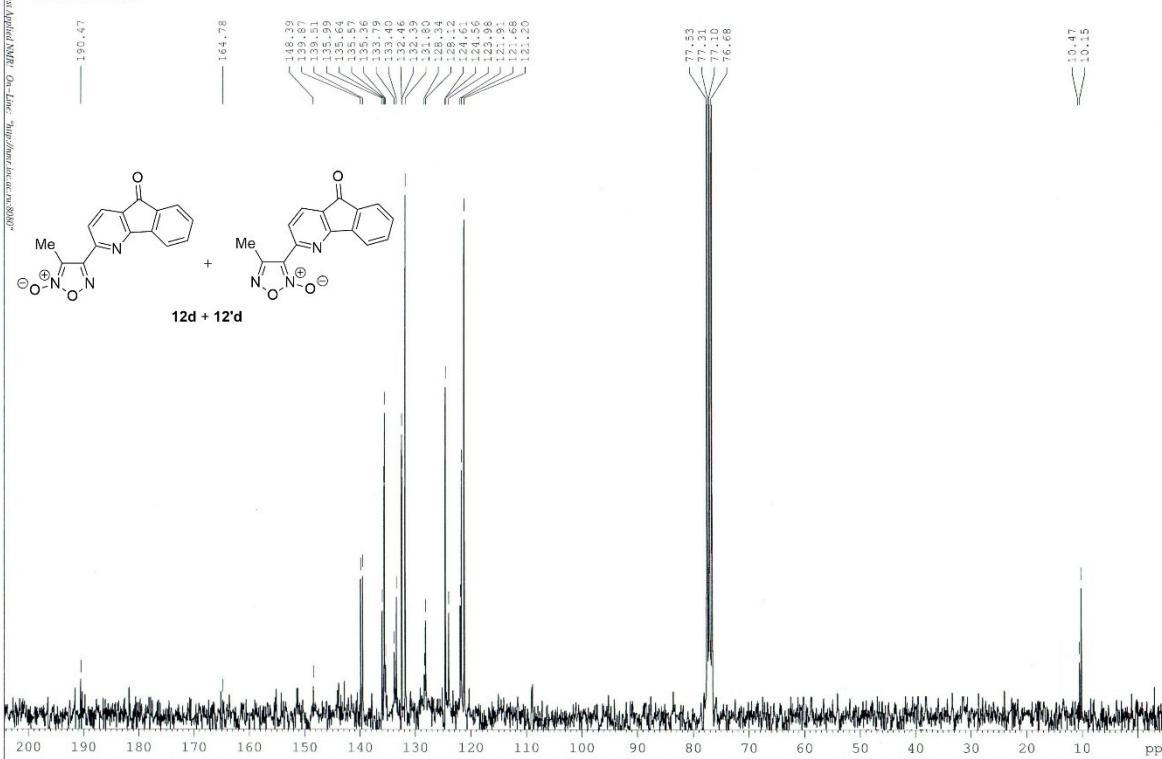
^{13}C NMR (50.3 MHz, CDCl_3) of a mixture **12c + 12'c**

/USED L093



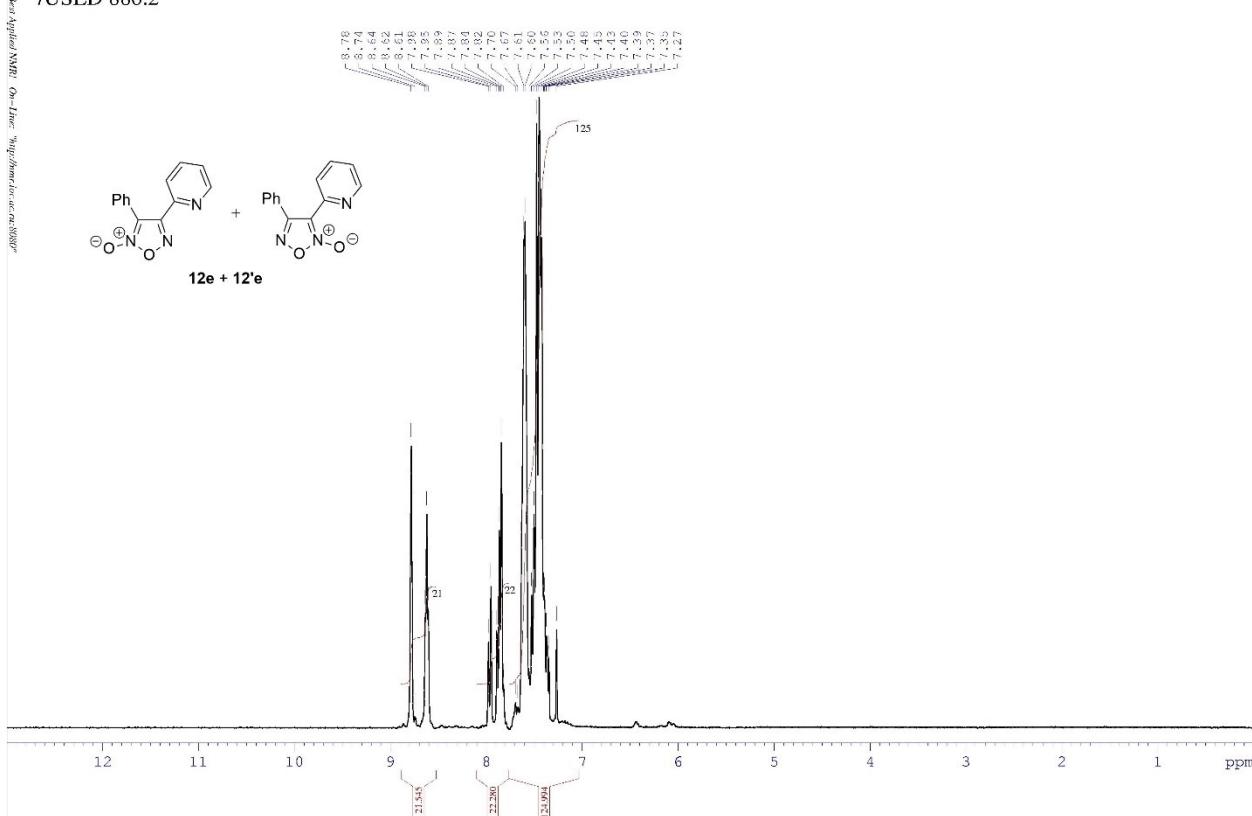
^1H NMR (200 MHz, CDCl_3) of a mixture **12d + 12'd**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=1.00 NS=274 SR=5.61 TE=300K 16 January 2016 Opr: Struchkova M.I.; Solv: CDCl₃; /USED L093



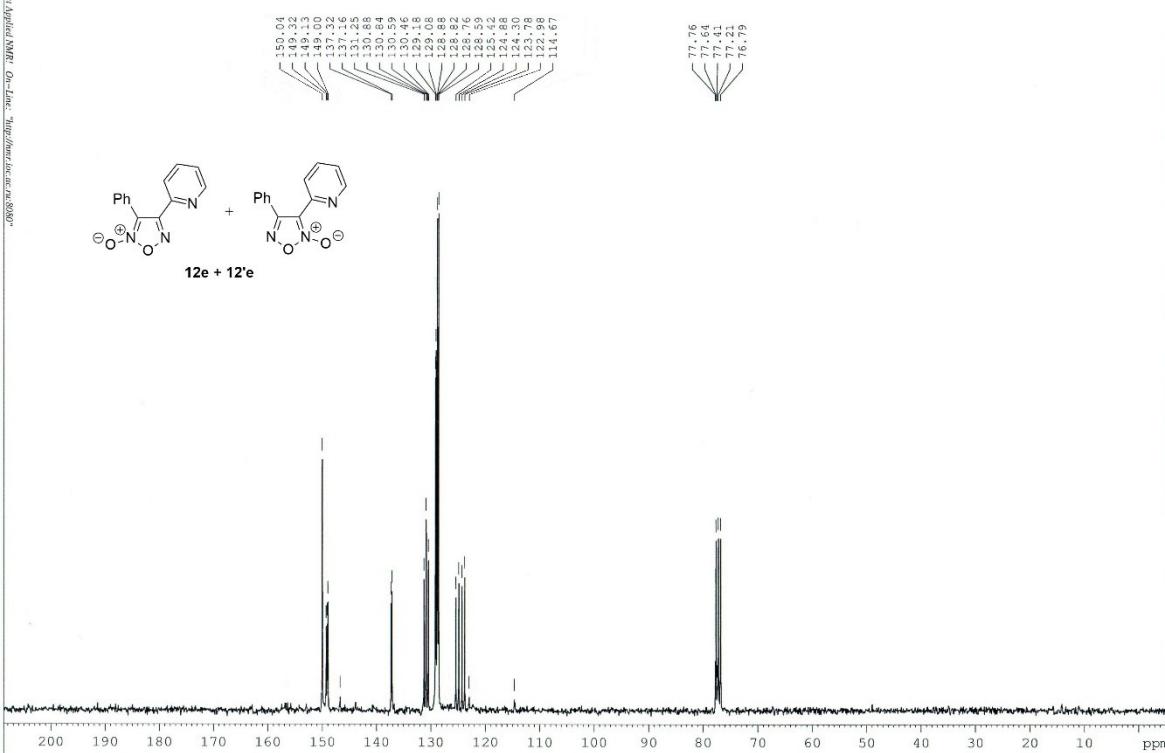
¹³C NMR (75.5 MHz, CDCl₃) of a mixture **12d + 12'd**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 NS=1 SR=4.18 TE=298K 18 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 886.2



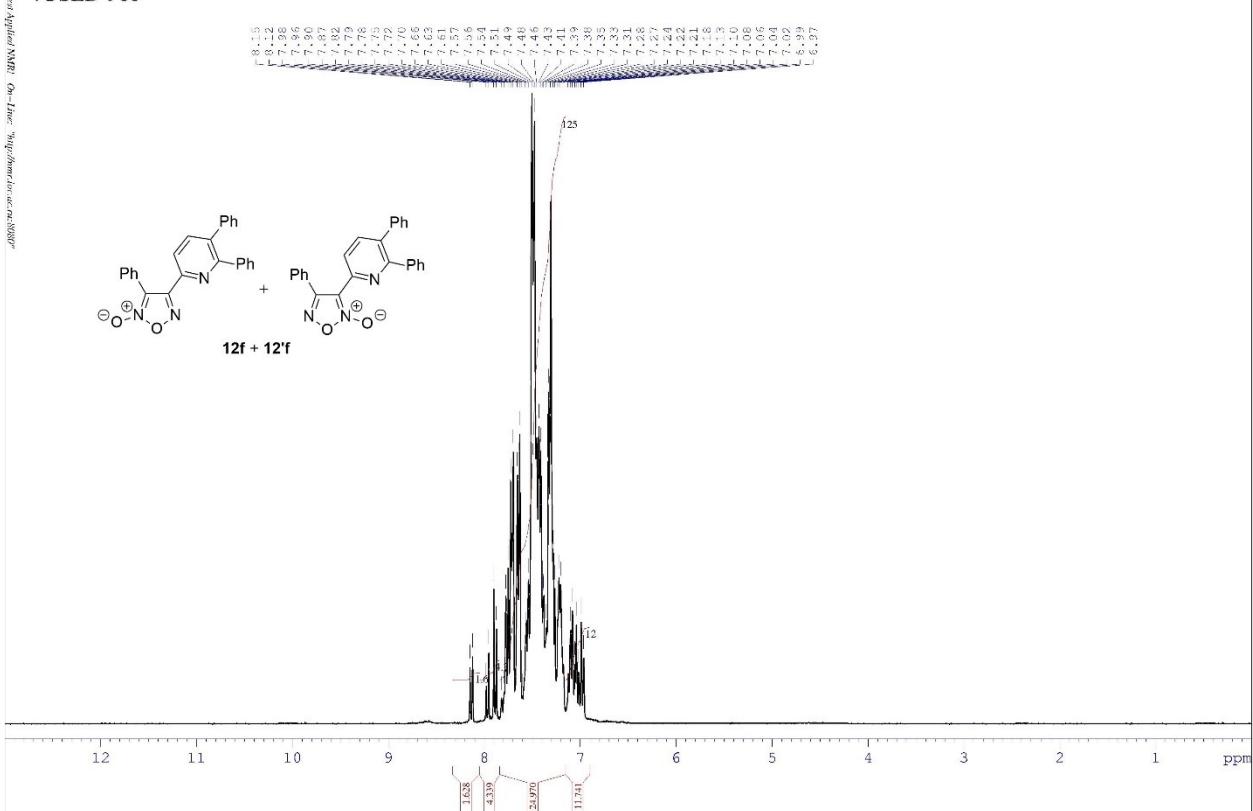
¹H NMR (300 MHz, CDCl₃) of a mixture **12e + 12'e**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=0.0 AQ=0.868 RD=1.00 NS=177 SR=-5.60 TE=300K 22 December 2015 Opr: Struchikova M.I.; Solv: CDCl₃; /USED 886.2



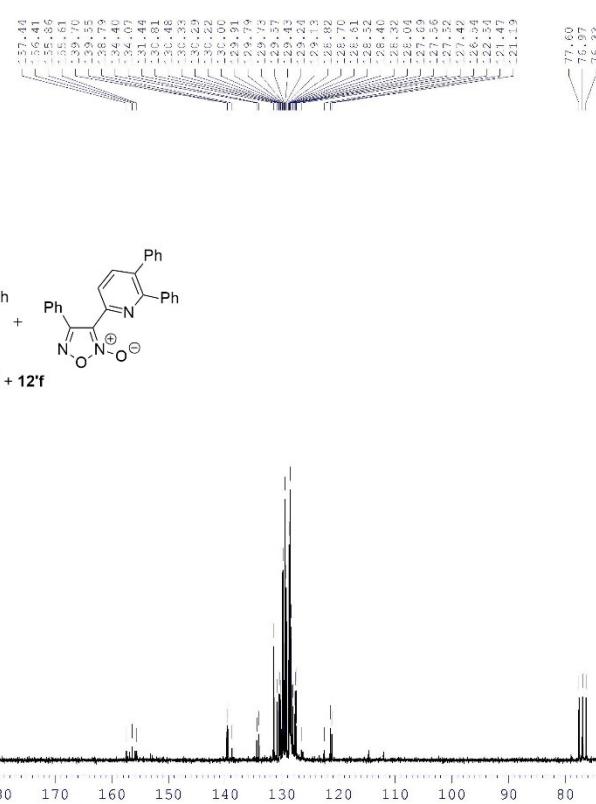
¹³C NMR (75.5 MHz, CDCl₃) of a mixture **12e + 12'e**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H}; SI=16K SW=7500 O1=2401 PW=9.0AQ=1.083 RD=2.00 NS=1 SR=4.17 TE=299K 3 February 2016 Opt: Struchkova M.I.; Solv: CDCl3;



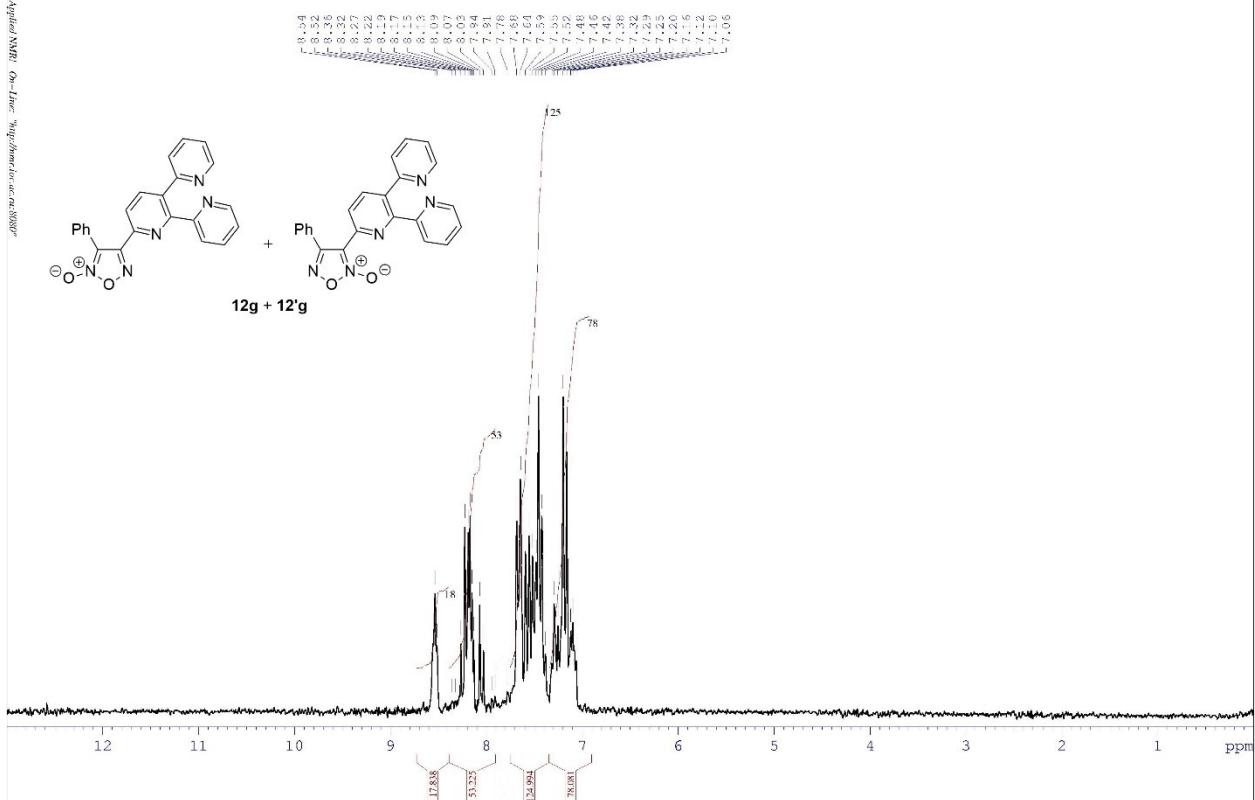
¹H NMR (300 MHz, CDCl₃) of a mixture **12f + 12'f**

/USED 900.C13

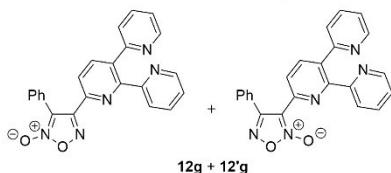


¹³C NMR (50.3 MHz, CDCl₃) of a mixture **12f + 12'f**

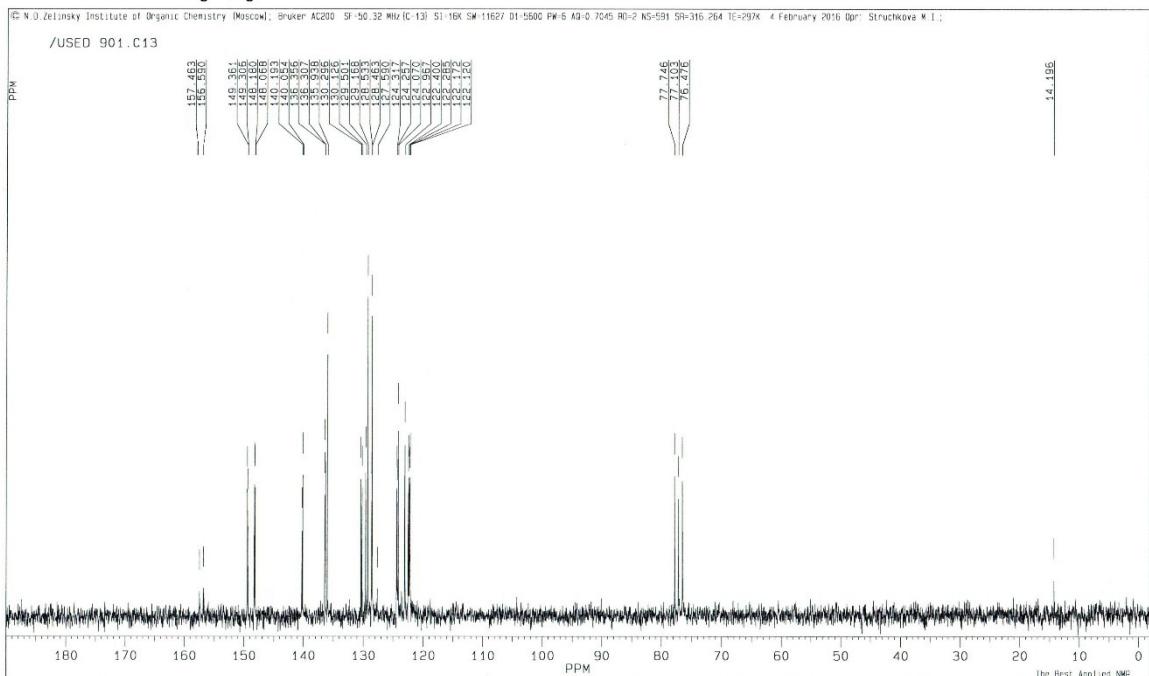
/USED 901



¹H NMR (200 MHz, CDCl₃) of a mixture **12g + 12'g**

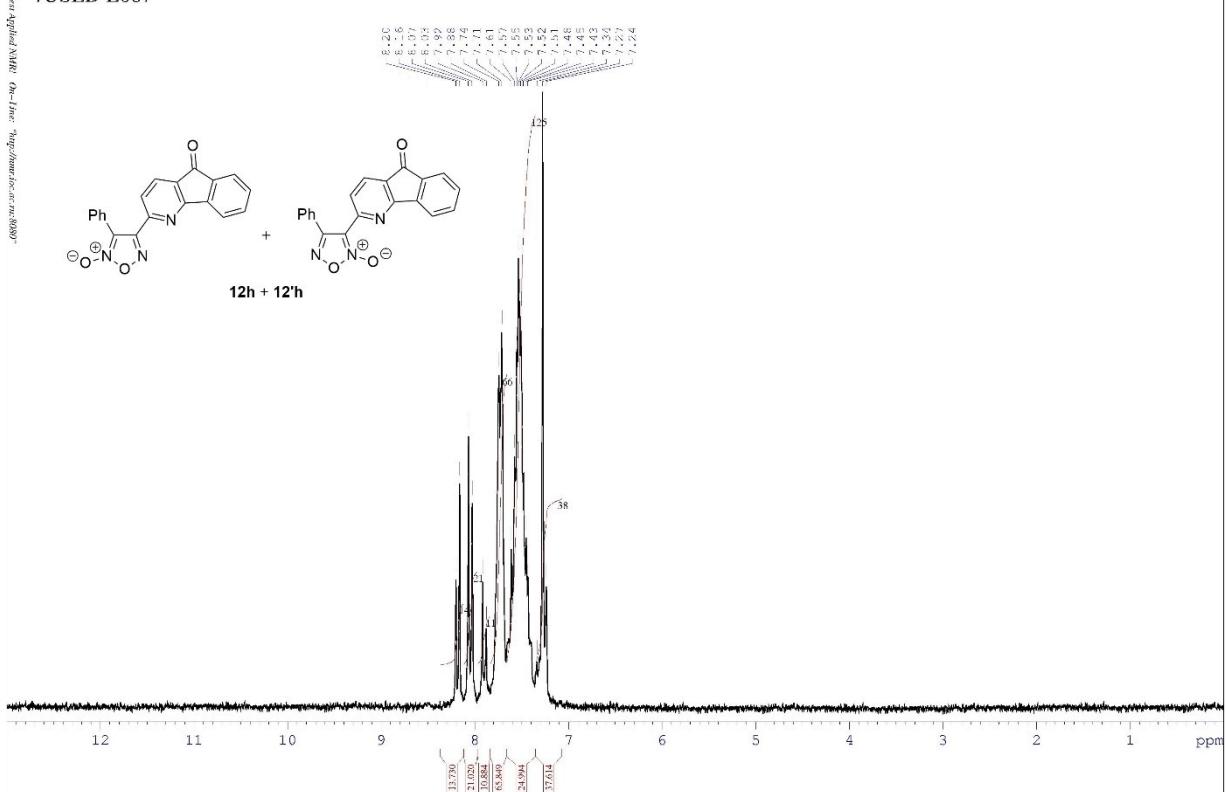


12g + 12'g

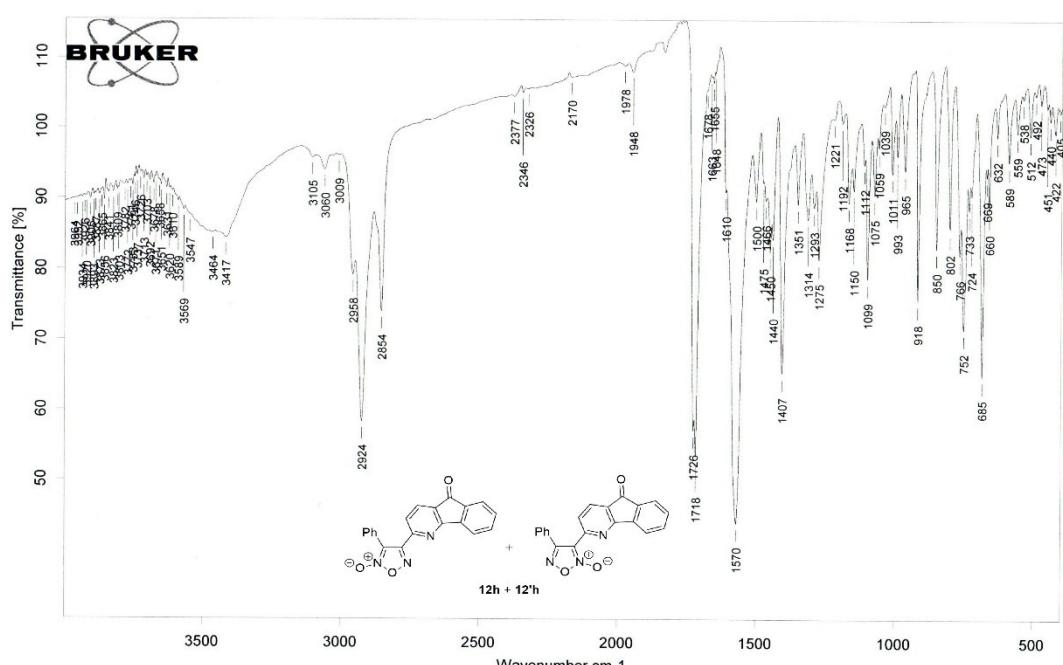
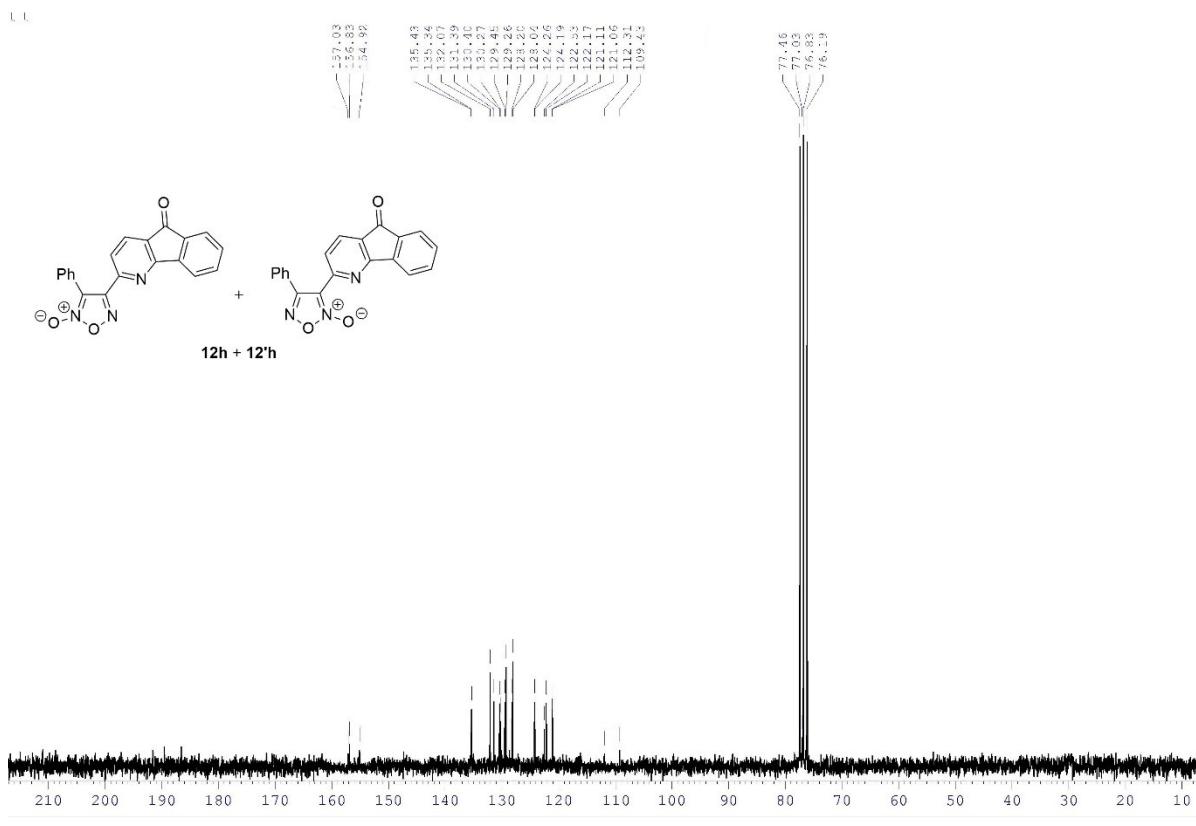


¹³C NMR (50.3 MHz, CDCl₃) of a mixture 12g + 12'g

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AC200 SF=200.13 MHz (1H) S1=16K SW=4000 O1=3939 PW=6.0 AQ=2.048 RD=3.00 NS=32 SR=2338.00 TE=297K 17 December 2015 Opr: Struchkova M.I.; Solv: CDCl₃; /USED L087



¹H NMR (200 MHz, CDCl₃) of a mixture 12h + 12'h

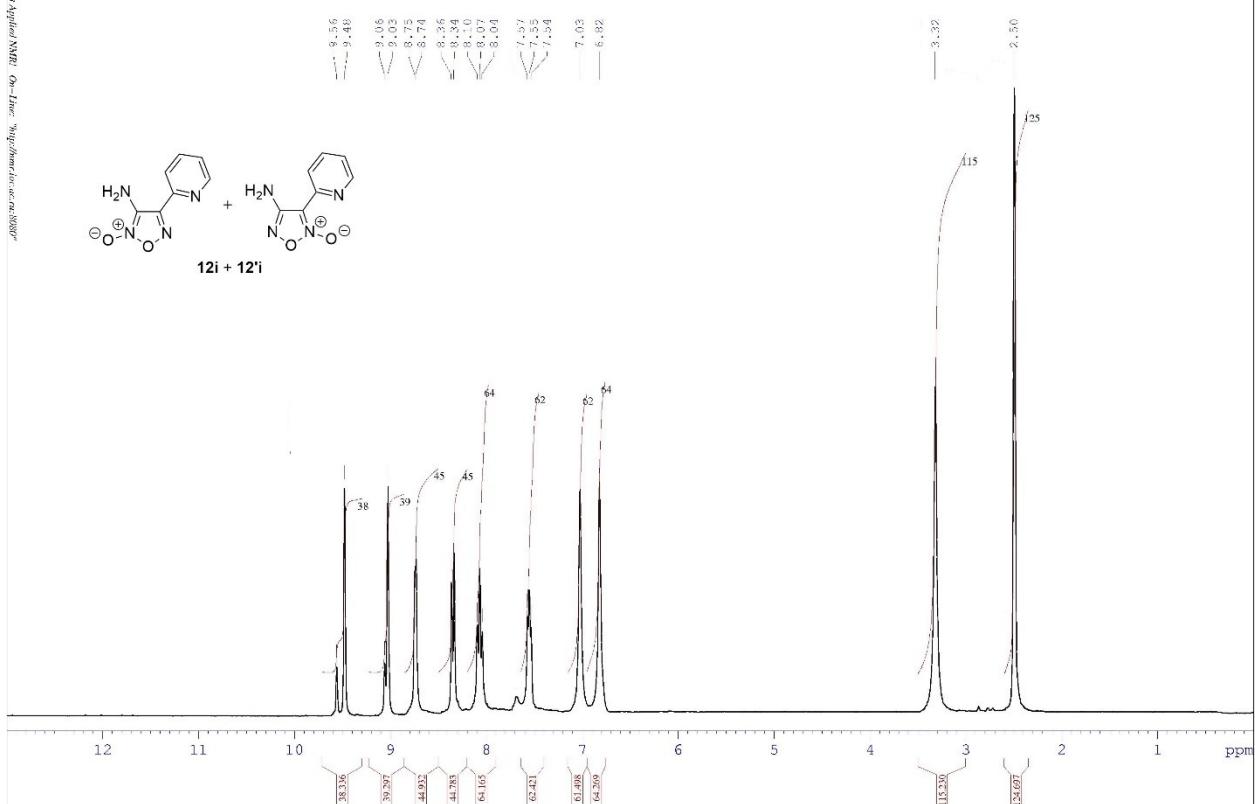


D:\EDL\87.0 ФЕРШТАТ. L-87, прессовка с KBr, 1/200.

21.01.2016

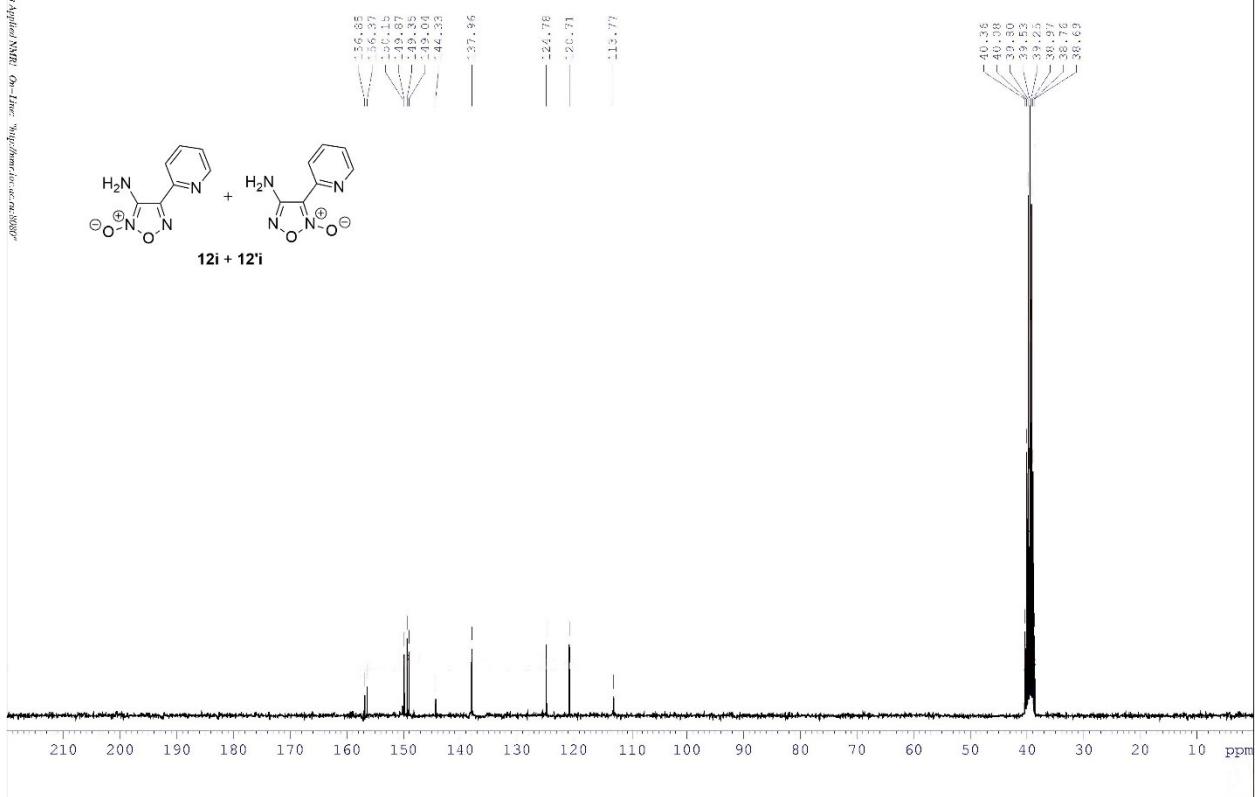
IR (KBr) of a mixture **12h + 12'h**

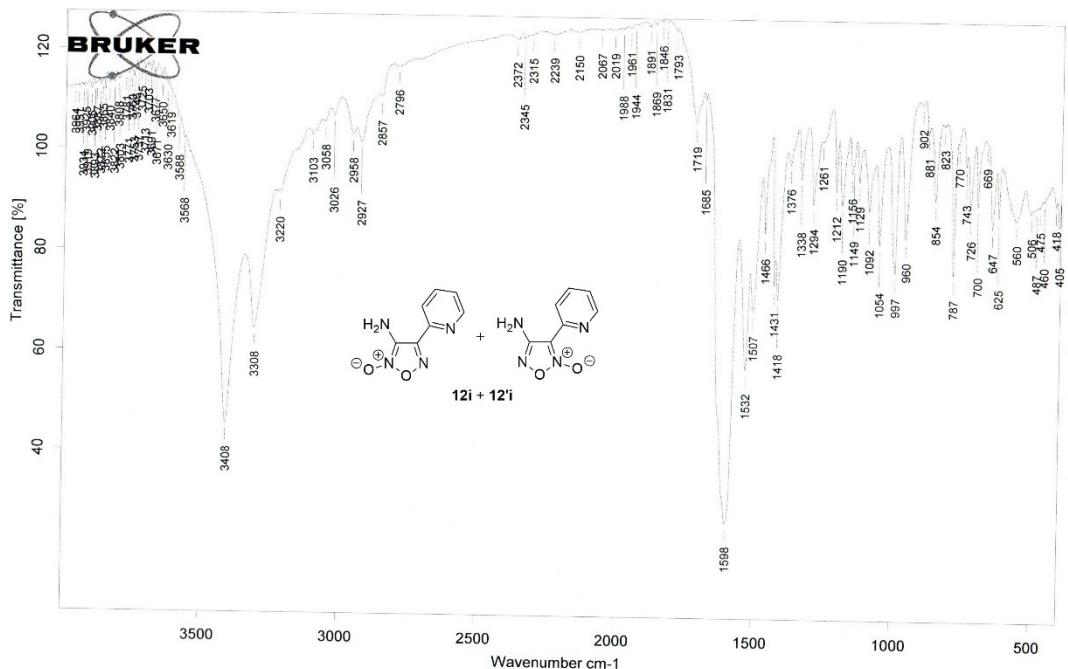
/USED 885.2



¹H NMR (300 MHz, DMSO-d₆) of a mixture **12i + 12'i**

/USED 885.2





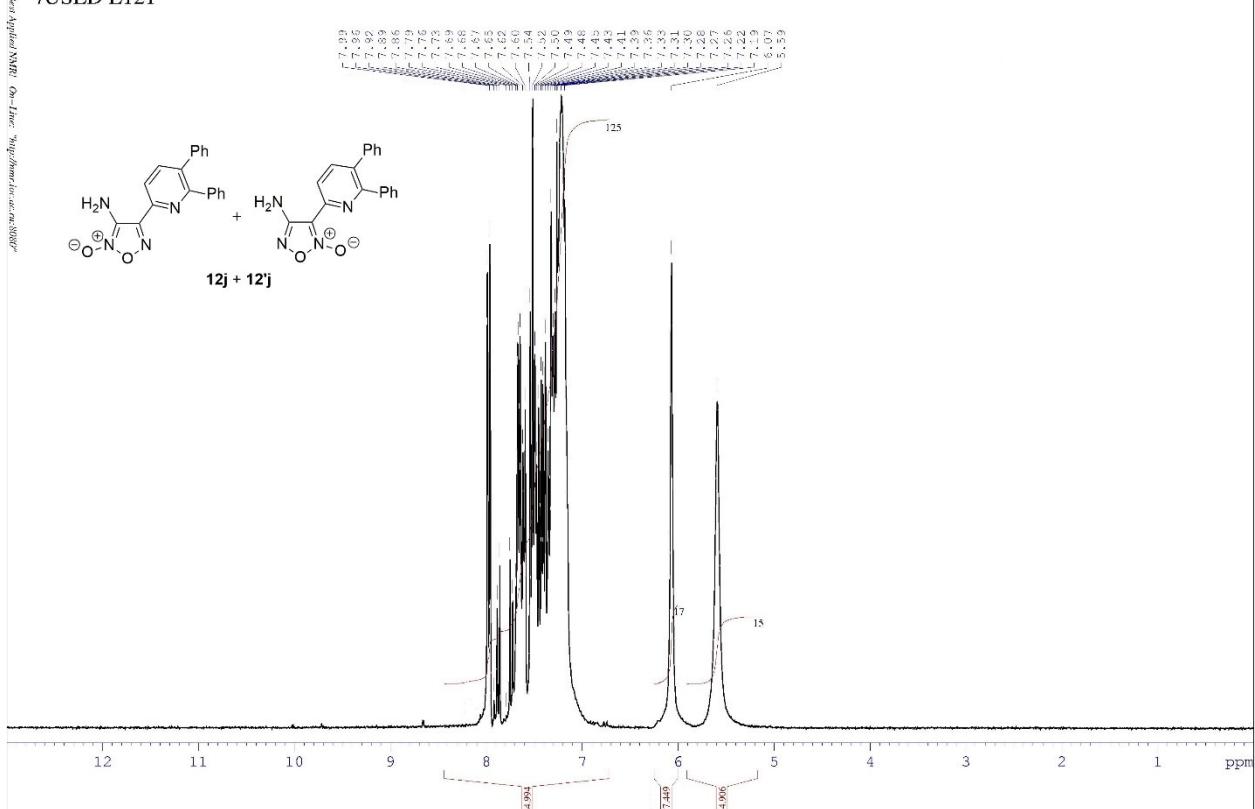
D:\EDL\LEO-885.0 ФЕРШТАТ . LEO-885 . прессовка с KBr, 1/200.

19.01.2016

Page 1/1

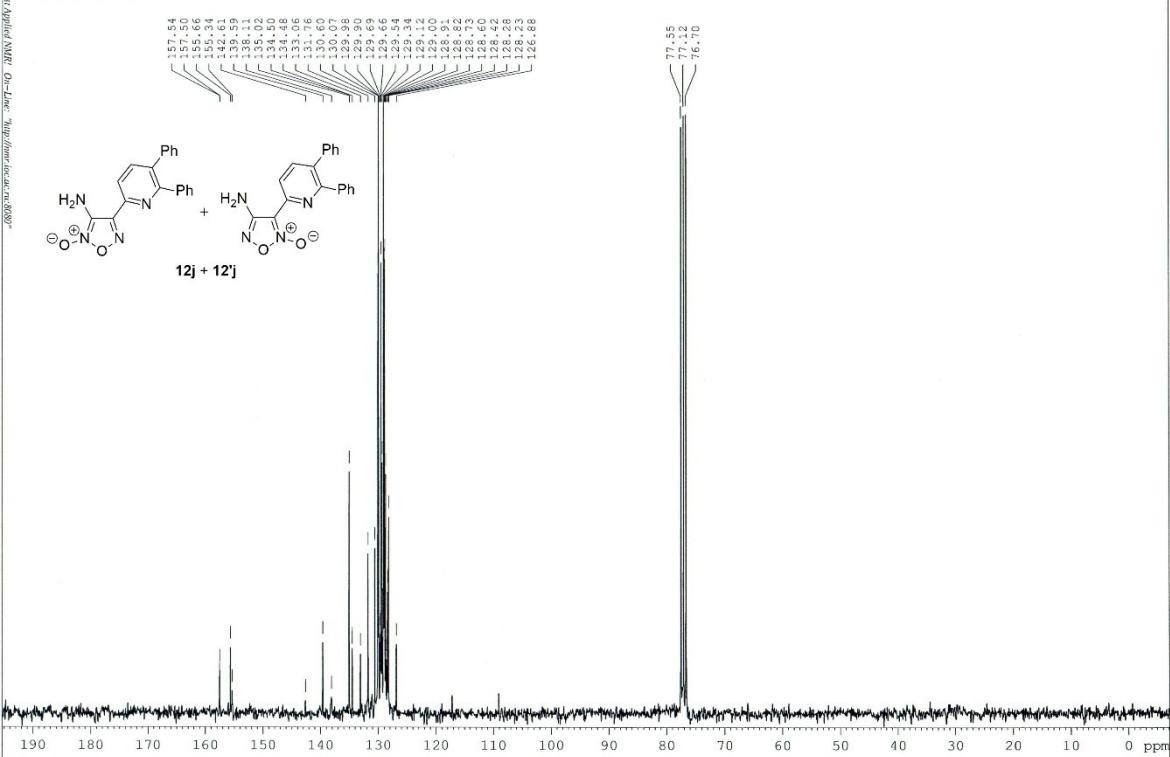
IR (KBr) of a mixture **12i + 12'i**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 N8=1 SR=4.16 TE=298K 29 January 2016 Opt: Struchkova M.I.; Solv: CDCl₃;
/USED L121

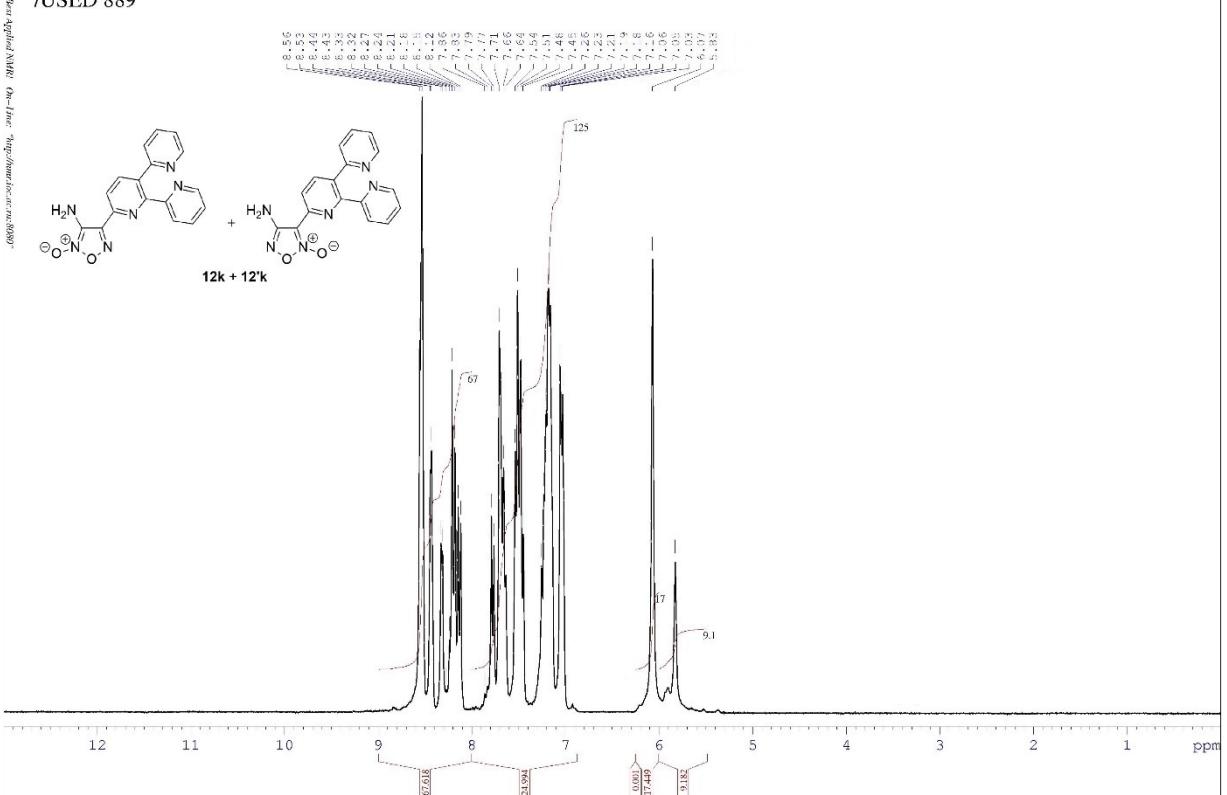


¹H NMR (300 MHz, CDCl₃) of a mixture **12j + 12'j**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {¹³C} SI=32K SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=1.00 NS=174 SR=5.61 TE=300K 1 February 2016 Opr: Struchkova M.I.; Solv: CDCl₃; /USED L121

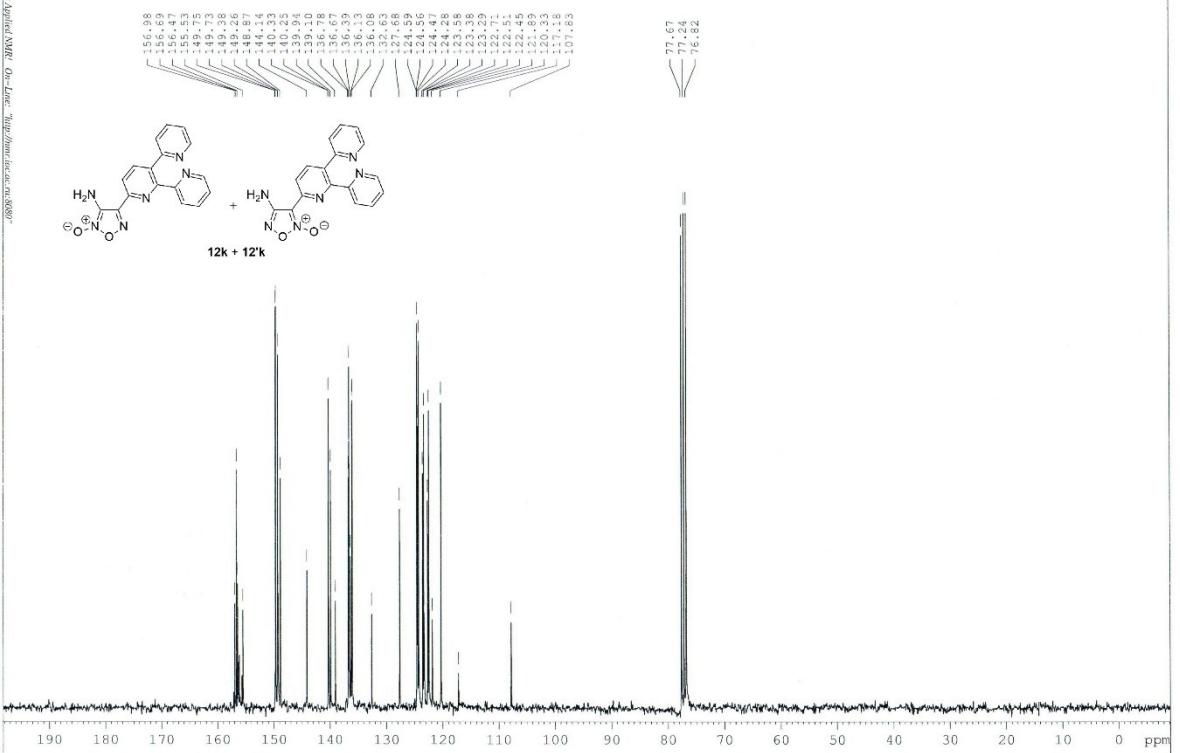


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {¹H} SI=16K SW=7500 O1=2401 PW=9.0 AQ=1.083 RD=2.00 NS=1 SR=4.16 TE=299K 20 January 2016 Opr: Struchkova M.I.; Solv: CDCl₃; /USED 889



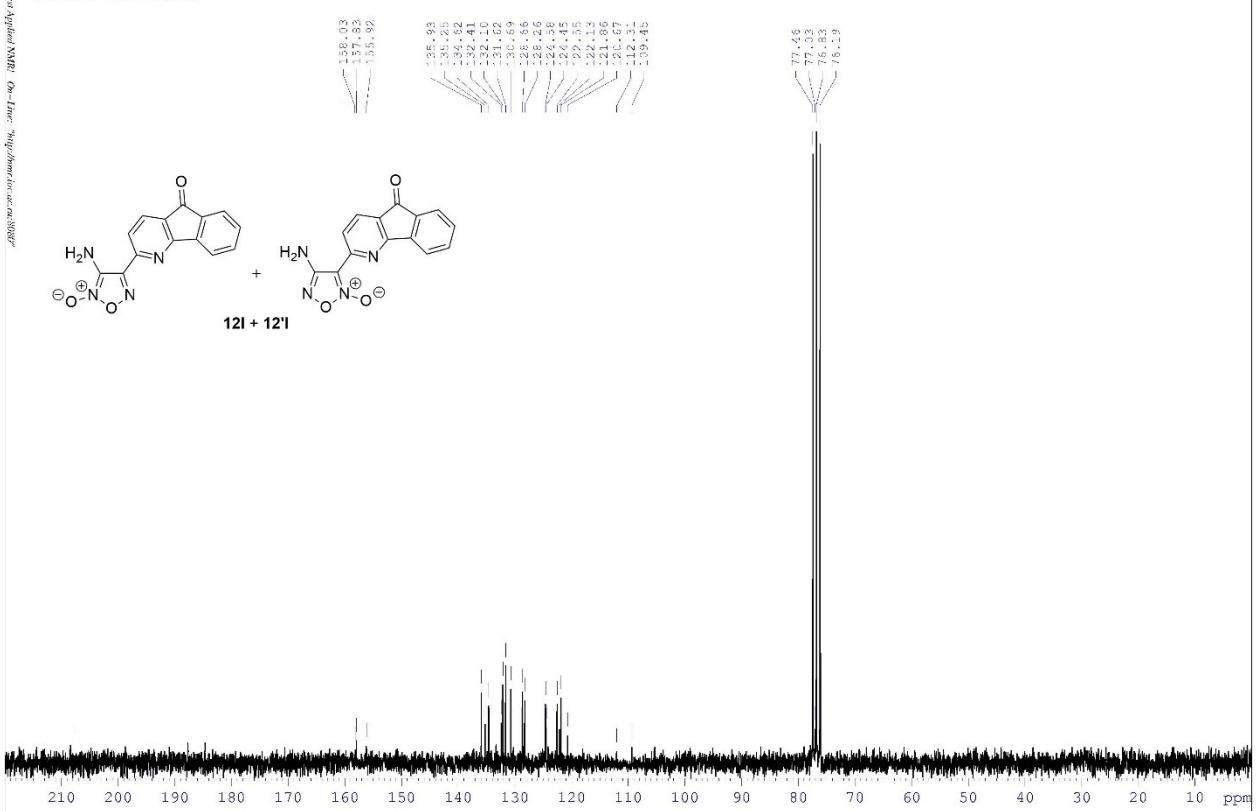
¹H NMR (300 MHz, CDCl₃) of a mixture **12k + 12'k**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz [13C] SI=32k SW=18795 O1=7920 PW=10.0 AQ=0.868 RD=2.00 NS=135 SR=5.61 TE=299K 20 January 2016 Opr: Struchkova M.I., Solv: CDCl₃; /USED 889



¹³C NMR (75.5 MHz, CDCl₃) of a mixture **12k** + **12'k**

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AC200 SF=50.32 MHz [13C] SI=16K SW=11627 O1=5600 PW=6.0 AQ=0.705 RD=2.00 NS=17240 SR=324.84 TE=297K 2 February 2016 Opr: Struchkova M.I.; Solv: CDCl₃



¹³C NMR (50.3 MHz, CDCl₃) of a mixture **12l + 12'l**