Supplementary Information for

An isoxazole strategy for the synthesis of alkyl 5-amino-4-cyano-1*h*-pyrrole-2-carboxylates – versatile building blocks for assembling pyrrolo-fused heterocycles

Anastasiya V. Agafonova, Liya D. Funt, Mikhail S. Novikov and Alexander F. Khlebnikov*

St. Petersburg State University, Institute of Chemistry, 7/9 Universitetskaya nab., St. Petersburg, 199034 Russia

*E-mail: a.khlebnikov@spbu.ru

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1. Computational details

All calculations were performed by using the Gaussian 16 suite of quantum chemical programs[1] at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of molecules were performed with the B3LYP[2]-D3[3] density functional method and 6-311+G(d,p) basis set using SMD[4] solvent model. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequency for the transition state was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Table S1. B3LYP-D3/6-311+G(d,p), SMD solvent model for 1,4-dioxane.

Absolute Energies (au), Cartesian Coordinates of stationary points
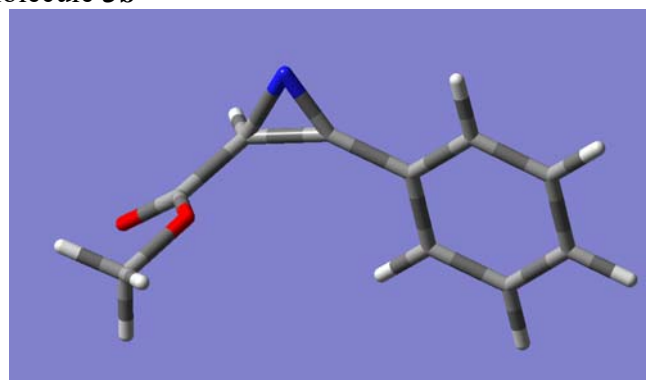
Molecule **4**				Molecule **3b**			

Molecule **4**
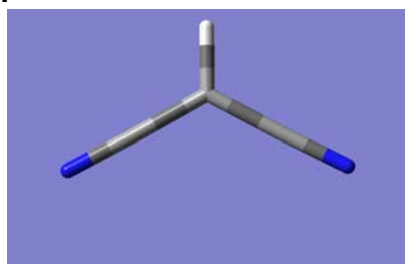
E = --224.552857, H (0K) = -224.521324,
H (298K) = -224.515742,
G (298K) = -224.548630 au.
Imaginary frequency = 0.

|			
C	1.2185480	0.0540320	-0.0001770
N	2.2581960	-0.4853280	0.0001020
C	-1.2185390	0.0540120	0.0000020
N	-2.2582150	-0.4853090	0.0000180
C	0.0000080	0.7233120	-0.0000130
H	0.0000370	1.8063190	0.0002890

Molecule **3b**

E = -591.816558, H (0K) = -591.647108,
H (298K) = -591.634502,
G (298K) = -591.686573 au.
Imaginary frequency = 0.

C	-0.0440690	1.0059010	-0.2802810
N	-0.7498180	1.9692060	0.1026070
C	-2.4244840	0.0269520	-0.4252200
C	1.2522750	0.3861590	-0.1420650
O	-3.3016780	-0.4004380	-1.1441760
C	2.2153660	0.9525080	0.7073740
C	3.4578230	0.3460490	0.8365840
C	3.7448850	-0.8211510	0.1234350
C	2.7885560	-1.3850690	-0.7207160
C	1.5408380	-0.7840660	-0.8550250
O	-2.2872360	-0.3008180	0.8706080
C	-3.2779440	-1.2005460	1.4074750
H	1.9785940	1.8569350	1.2559530
H	4.2047310	0.7787560	1.4921010
H	4.7165420	-1.2907850	0.2279940
H	3.0150360	-2.2905260	-1.2715530
H	0.7873420	-1.2120970	-1.5065390
H	-3.2559250	-2.1553480	0.8787450
H	-4.2751510	-0.7642630	1.3270770
H	-3.0083960	-1.3392320	2.4527860
C	-1.3669400	0.9616870	-0.8971810
H	-1.5205830	1.3116290	-1.9125470

TS[4-5]	Molecule **5**
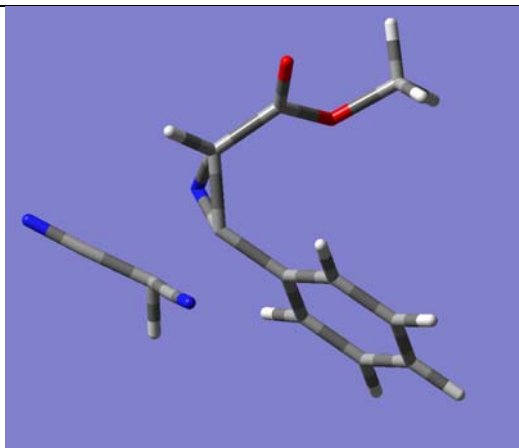
E = -816.354397, H (0K) = -816.151820,			
H (298K) = -816.134562,			
G (298K) = -816.196939 au.			
Imaginary frequency = 1.			
C	-3.3173110	-0.3626180	-0.5453570
C	-0.6840100	0.0184320	-0.6014470
N	-0.8409410	0.8521690	-1.6427840
C	0.2631680	2.2679980	0.2353630
C	0.5152320	-0.8411040	-0.3441640
O	0.1760020	3.0290780	1.1842090
N	-4.2581260	0.1874630	-0.9291150
C	-2.1074110	-1.3142750	1.2894410
N	-2.0470580	-1.5447550	2.4222470
C	1.0907030	-1.5317130	-1.4145420
C	2.2124290	-2.3334030	-1.2185160
C	2.7810860	-2.4436140	0.0521780
C	2.2182870	-1.7481230	1.1217840
C	1.0872480	-0.9556730	0.9260830
O	1.4249360	2.0734180	-0.4290660
C	2.5736500	2.7343040	0.1124740
H	0.6657370	-1.4077150	-2.4047420
H	2.6518490	-2.8625580	-2.0580650
H	3.6601040	-3.0611870	0.2045750
H	2.6589900	-1.8215000	2.1105740
H	0.6525030	-0.4141640	1.7582130
H	2.7711320	2.3986440	1.1340600
H	2.4417590	3.8191830	0.1142980
H	3.4043640	2.4584220	-0.5366010
C	-2.0955760	-0.9965000	-0.1165170
H	-1.9216690	-1.8999350	-0.7051080
C	-0.8640140	1.4603830	-0.2906430
H	-1.8102930	1.7821480	0.1523990

TS⁵⁻⁷
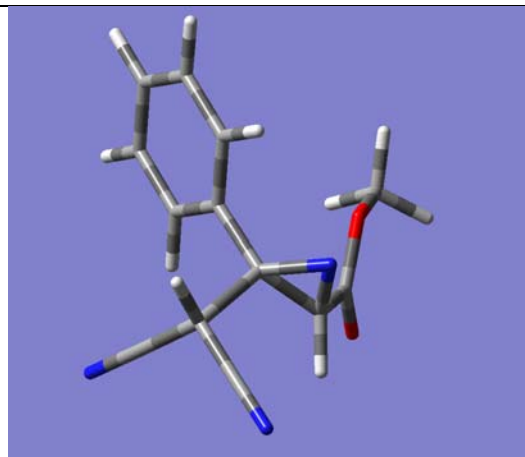
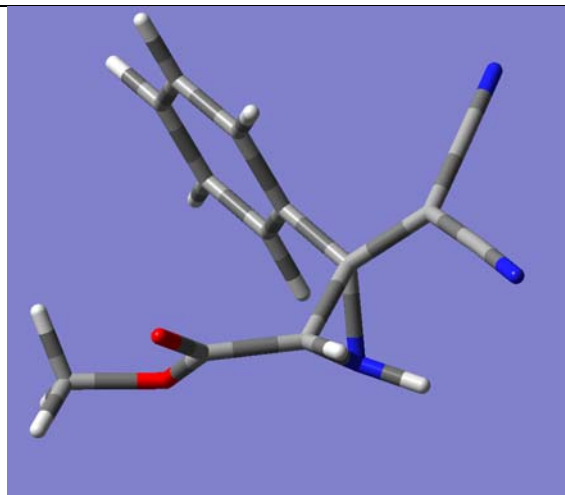|			
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H (298K) = -816.133788,			
G (298K) = -816.197354 au.			
Imaginary frequency = 0.			
C	3.3232020	0.2478790	-0.5364390
C	0.7409750	-0.0048290	-0.5870000
N	0.8613770	-0.8807300	-1.6328900
C	-0.2832390	-2.2168230	0.2816790
C	-0.4931250	0.8283300	-0.3418110
O	-0.2075300	-2.9487780	1.2548340
N	4.2982270	-0.3107280	-0.7969150
C	2.1264320	1.4128380	1.1661060
N	2.1043000	1.7633460	2.2672050
C	-1.1363930	1.4142360	-1.4357730
C	-2.2891670	2.1755830	-1.2571000
C	-2.8233460	2.3490320	0.0215580
C	-2.1938570	1.7583050	1.1165230
C	-1.0318290	1.0078170	0.9358200
O	-1.4440690	-2.0198330	-0.3813300
C	-2.6043760	-2.6327430	0.1897150
H	-0.7395110	1.2356580	-2.4291210
H	-2.7802840	2.6228240	-2.1155550
H	-3.7269720	2.9333900	0.1612130
H	-2.6070870	1.8791380	2.1126410
H	-0.5497440	0.5448790	1.7890930
H	-2.7816350	-2.2652230	1.2039490
H	-2.5029660	-3.7206690	0.2189220
H	-3.4341810	-2.3507640	-0.4580500
C	2.0839300	0.9360200	-0.2074810
H	1.9801830	1.7973720	-0.8751490
C	0.8657220	-1.4611110	-0.2834030
H	1.7980970	-1.8181320	0.1678590

Molecule **7**

S3
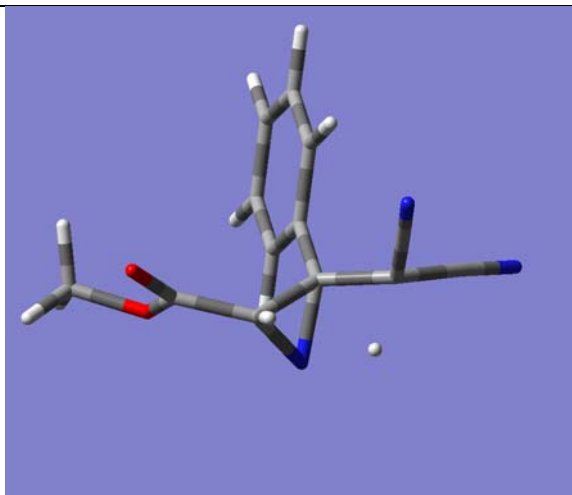
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C	2.6919650	-1.3033650	0.8396660
C	0.6187330	-0.4642730	-0.4397860
N	0.2793260	-1.2154430	-1.6514660
C	-1.5269040	-1.8246340	0.1042330
C	0.0189140	0.8486820	-0.0539110
O	-1.8971930	-2.4972760	1.0480260
N	3.1112580	-1.8562610	1.7690940
C	2.9515830	0.3853280	-0.8504540
N	3.5850320	1.2341550	-1.3193260
C	-0.8329700	1.5213480	-0.9341320
C	-1.3915430	2.7468440	-0.5786100
C	-1.1059980	3.3166430	0.6627850
C	-0.2522940	2.6532270	1.5447230
C	0.3083850	1.4286240	1.1873190
O	-2.3619890	-1.0427280	-0.6047340
C	-3.7045810	-0.9431840	-0.1102310
H	-1.0504370	1.0564850	-1.8874420
H	-2.0488690	3.2605990	-1.2728920
H	-1.5402350	4.2718850	0.9389760
H	-0.0203300	3.0901010	2.5104520
H	0.9725140	0.9175380	1.8767690
H	-3.7141490	-0.5439350	0.9067130
H	-4.1985910	-1.9175940	-0.1179890
H	-4.2144160	-0.2571680	-0.7857820
C	2.1493240	-0.6866920	-0.3340840
H	1.7510530	-1.4276820	-1.3433520
C	-0.1124510	-1.7847460	-0.3727750
H	0.4346110	-2.6301660	0.0516240

| C	2.6424250	1.4454460	-0.0032240
C	0.8312780	-0.2570360	-0.3891090
C	-0.9675610	-2.0266220	0.2782220
C	-0.2000500	0.8168220	-0.1557980
O	-1.1618030	-2.5216610	1.3706990
N	2.9799440	2.5641590	0.0067500
C	3.1859260	-0.8826240	0.2287640
N	3.9505100	-1.7496530	0.4080880
C	-0.9466930	1.3490690	-1.2069870
C	-1.9030740	2.3340950	-0.9652680
C	-2.1311070	2.7883740	0.3329530
C	-1.3894430	2.2563820	1.3886310
C	-0.4262460	1.2812140	1.1440720
O	-1.9550040	-1.6760760	-0.5615230
C	-3.2913140	-1.8020120	-0.0482250
H	-0.7816380	0.9744890	-2.2093300
H	-2.4720520	2.7456120	-1.7926310
H	-2.8767050	3.5537470	0.5213000
H	-1.5565020	2.6053510	2.4021340
H	0.1603920	0.8756030	1.9607020
H	-3.4185550	-1.1817320	0.8415620
H	-3.5196350	-2.8412010	0.1987560
H	-3.9436150	-1.4504880	-0.8462230
C	2.2326000	0.1100200	0.0002830
C	0.3945810	-1.7042250	-0.2267780
H	1.1476550	-2.3797860	0.1655590
N	0.5753110	-1.1202390	-1.5632600
H	1.4668200	-1.4329860	-1.9414850

TS[7-8]	Molecule 8
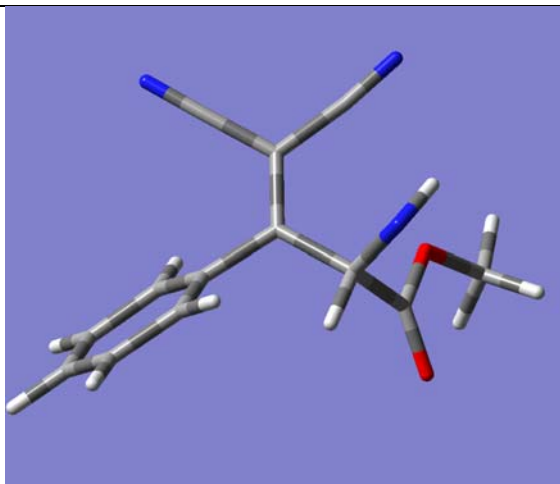
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G (298K) = -816.202093 au.
Imaginary frequency = 1.

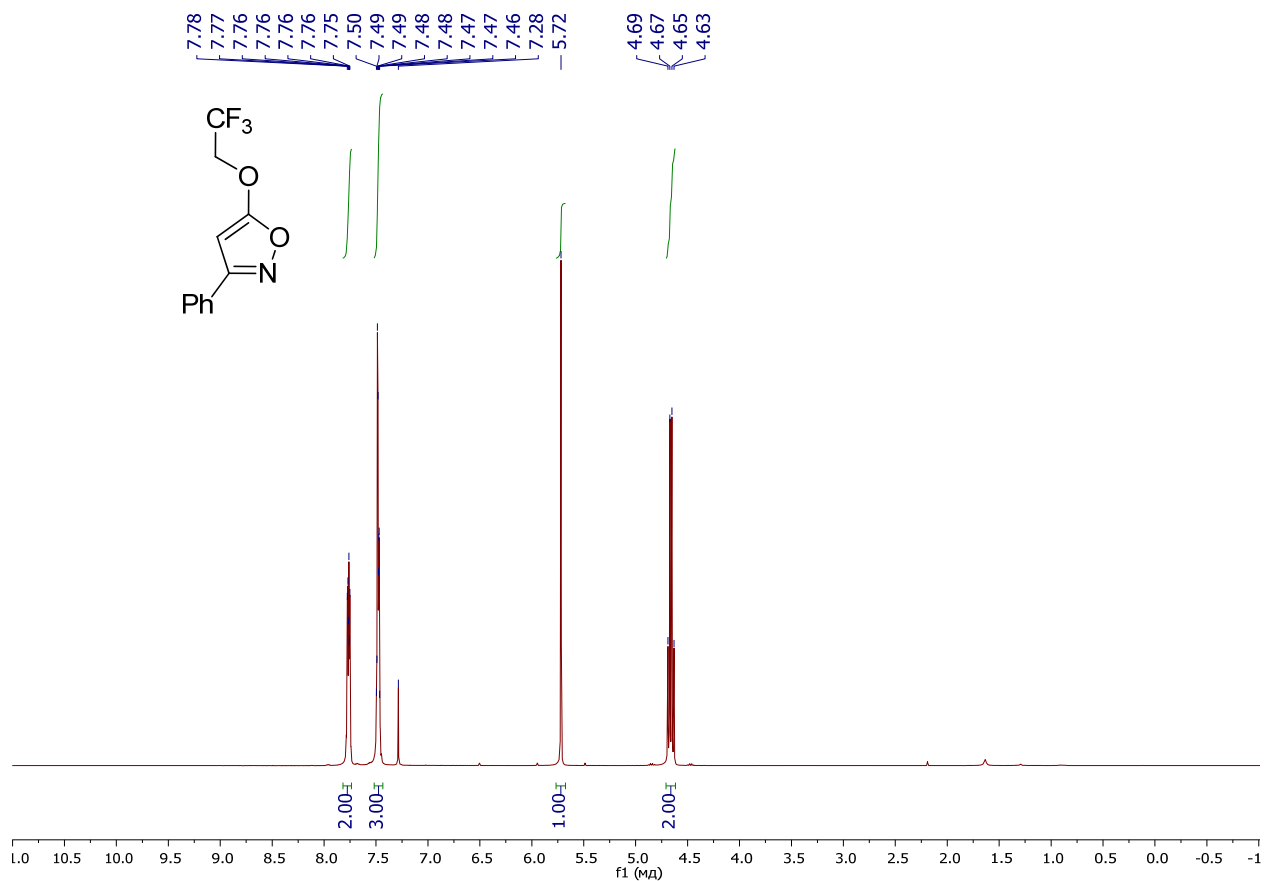|			
C	-0.5279370	2.5664600	-0.2379660
C	-0.0407450	0.2568780	0.4072020
C	1.7244780	-1.5183720	-0.0440860
C	-1.4423090	-0.1241990	0.1479720
O	1.7932410	-2.7138300	-0.2417610
N	-1.2430240	3.4099780	-0.5824900
C	1.7147880	2.0078870	0.3509590
N	2.7558930	2.5002830	0.4583000
C	-2.0082350	0.0335560	-1.1277700
C	-3.3071770	-0.3944770	-1.3838440
C	-4.0715490	-0.9696140	-0.3690330
C	-3.5218190	-1.1238870	0.9038850
C	-2.2162080	-0.7178430	1.1602120
O	2.4908680	-0.6257330	-0.7131460
C	3.4814510	-1.1630790	-1.6008730
H	-1.4200450	0.4780070	-1.9219260
H	-3.7233090	-0.2740860	-2.3781820
H	-5.0866300	-1.2953740	-0.5684020
H	-4.1107840	-1.5638140	1.7013910
H	-1.7970910	-0.8330270	2.1528680
H	3.0167700	-1.7522300	-2.3953850
H	4.1876650	-1.7924180	-1.0539380
H	3.9965890	-0.3005350	-2.0220600
C	0.3747450	1.5411550	0.1712070
C	0.8701440	-0.8460920	1.0396120
H	0.1693390	-1.6329990	1.3344920
N	1.6134240	-0.4379300	2.1826830
H	2.4328080	0.0864210	1.8760880
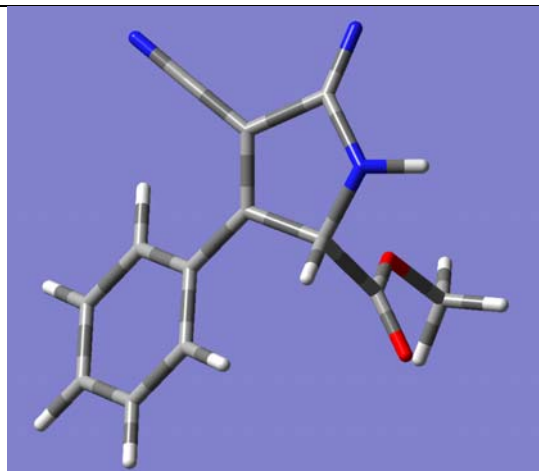
E = -816.389639, H (0K) = -816.182981,
H (298K) = -816.166131,
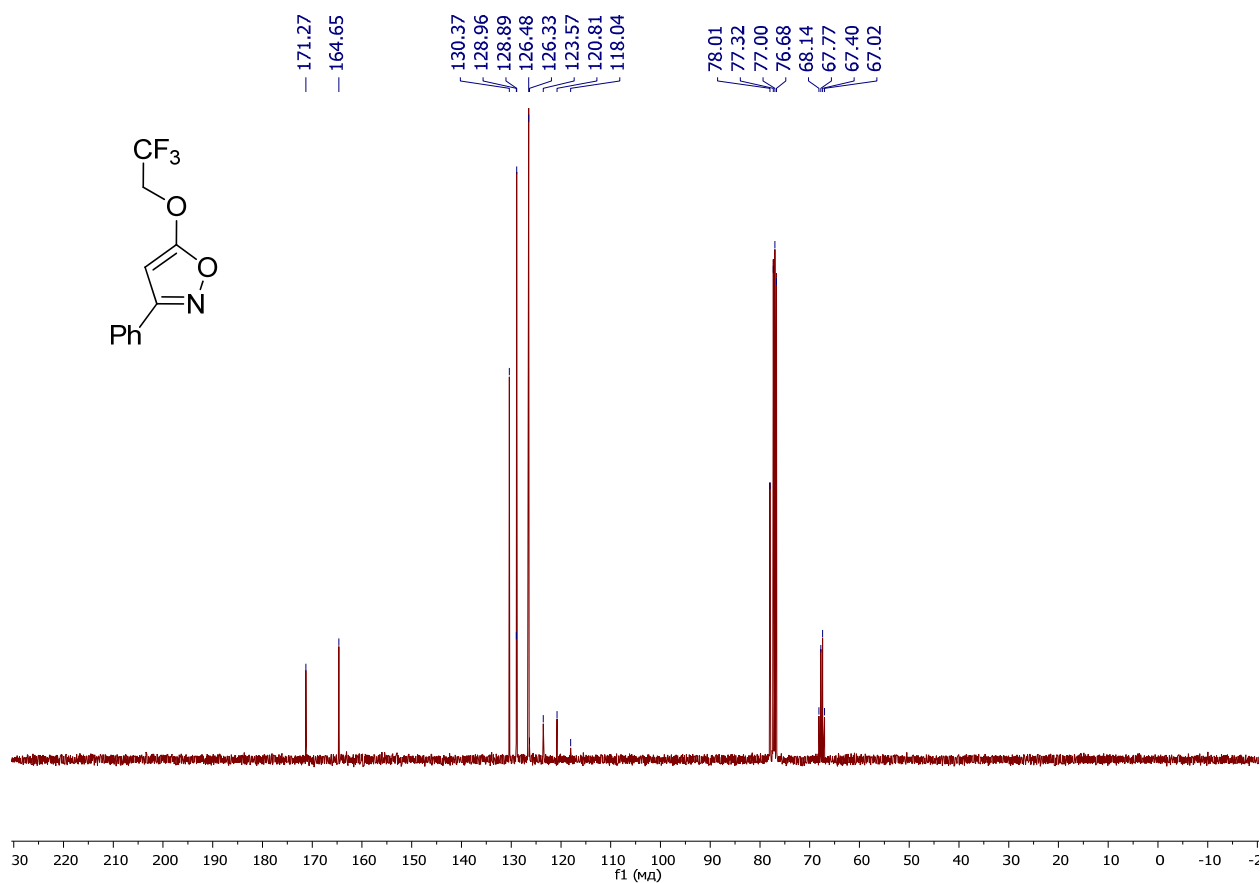G (298K) = -816.227544 au.
Imaginary frequency = 0.

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C	0.1771800	0.5038890	0.4753920
C	1.0126860	-1.8865810	0.2103110
C	-1.2622590	0.2977910	0.2907180
O	0.8746870	-3.0022400	0.6658440
N	0.1990350	3.8936020	-0.5964270
C	2.4592340	1.2542810	0.3333530
N	3.4418170	1.8438010	-0.1098910
C	-1.9952050	1.0132580	-0.6754960
C	-3.3560490	0.7922890	-0.8494990
C	-4.0259520	-0.1532770	-0.0709450
C	-3.3140140	-0.8796210	0.8816420
C	-1.9504440	-0.6612780	1.0580850
O	1.1934160	-1.6365330	-1.0960440
C	1.2542650	-2.7794160	-1.9668340
H	-1.4924360	1.7361100	-1.3041350
H	-3.8948050	1.3561610	-1.6034470
H	-5.0879860	-0.3240580	-0.2096750
H	-3.8195670	-1.6209420	1.4912880
H	-1.4215390	-1.2357460	1.8083580
H	0.3212620	-3.3455630	-1.9246830
H	2.0862110	-3.4304920	-1.6894150
H	1.4085590	-2.3761230	-2.9661680
C	0.9584200	1.5688770	0.1918720
C	1.0603420	-0.6083040	1.0488340
H	0.7117740	-0.9020800	2.0450910
N	2.3859210	-0.0104850	1.1151760
H	3.1637530	-0.6256570	0.9113910

2. NMR spectra of new compounds

^{1}H NMR spectra (CDCl$_3$, 400 MHz) of compound **1s**

7.78, 7.77, 7.76, 7.76, 7.76, 7.76, 7.75, 7.50, 7.49, 7.49, 7.48, 7.48, 7.47, 7.47, 7.46, 7.28, 5.72, 4.69, 4.67, 4.65, 4.63

2.00, 3.00, 1.00, 2.00

f1 (мд)

^{13}C NMR spectra (CDCl$_3$, 100 MHz) of compound **1s**

171.27, 164.65, 130.37, 128.96, 128.89, 126.48, 126.33, 123.57, 120.81, 118.04, 78.01, 77.32, 77.00, 76.68, 68.14, 67.77, 67.40, 67.02

f1 (мд)

S6

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **1t**
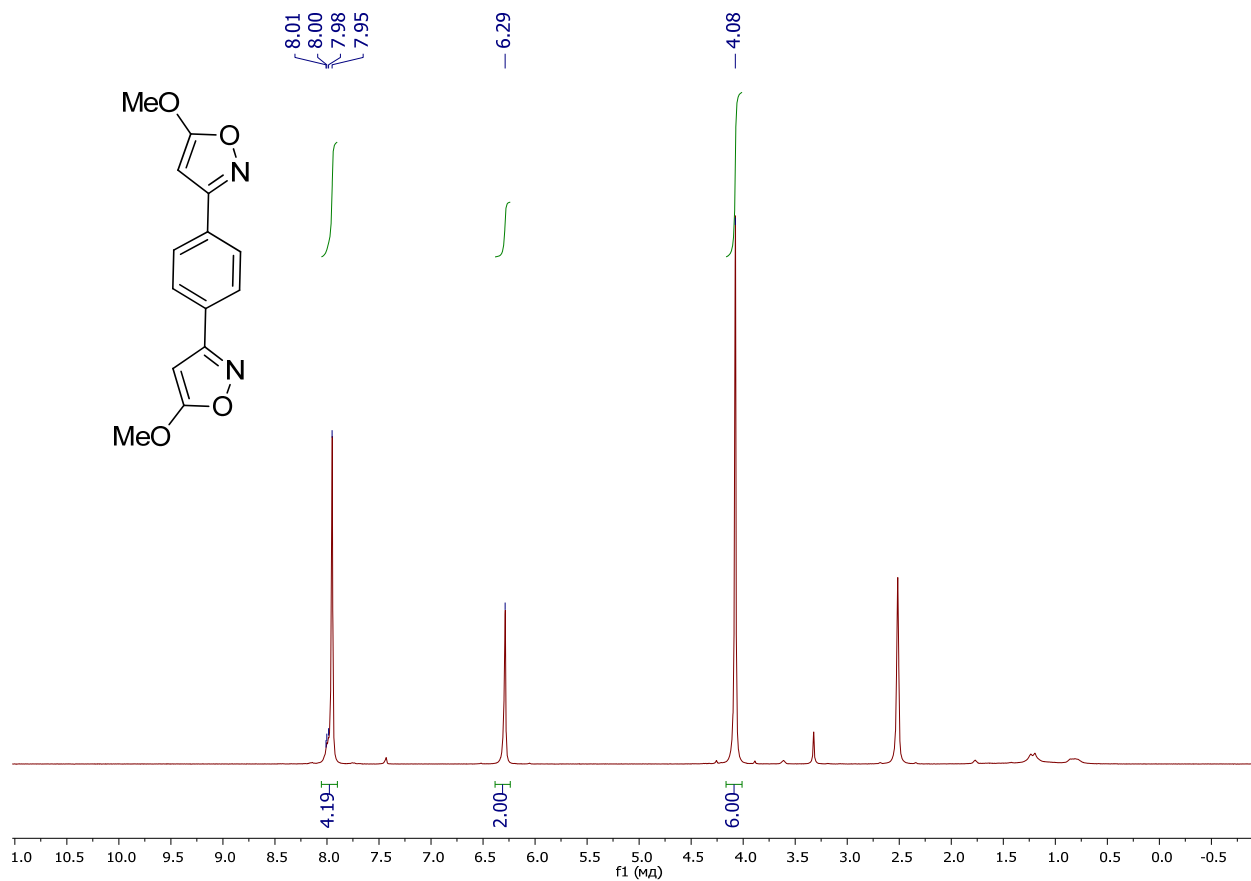
^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **1t**

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2a**

10.87

7.31
7.30
7.29
7.29
7.20
7.18

6.10

3.59

2.51
2.50
2.50
2.50
2.49
2.34

Me

CN

MeO$_2$C   NH$_2$
       N
       H

1.00

2.01
2.01

2.00

3.00

3.00

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2a**

159.76

149.37

137.01
133.17
129.42
129.31
128.21

116.42
109.41

75.51

50.72
40.13
39.92
39.71
39.50
39.29
39.08
38.87
20.80

Me

CN

MeO$_2$C   NH$_2$
       N
       H

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S8

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2b**

Peaks: 10.93; 7.43, 7.41, 7.39, 7.37, 7.36, 7.34; 6.13; 3.60; 2.50

Integrations: 0.96; 5.03; 1.97; 3.00

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2b**

Peaks: 159.69; 149.40; 133.07, 132.25, 129.53, 127.67, 127.59, 116.34; 109.55; 75.49; 50.75, 40.13, 39.92, 39.71, 39.50, 39.29, 39.08, 38.87

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2c

10.88

7.42
7.40
7.37
7.35

6.11

3.61

2.50

1.31

0.97

4.01

1.95

3.00

9.04

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2c

159.63

150.08
149.40

133.13
129.22
124.36
116.51
109.33

75.44

50.72
40.12
39.92
39.71
39.50
39.29
39.09
38.88
34.30
31.05

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (мд)

S10

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2d**

10.84

7.36
7.35
6.96
6.94

6.10

3.79
3.60

2.50

1.00

2.03
2.01

2.01

3.08
3.02

2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2d**

159.76
158.86
149.32
133.07
130.78
124.38
116.51
113.08
109.24

75.47

55.05
50.70
40.13
39.92
39.71
39.50
39.30
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
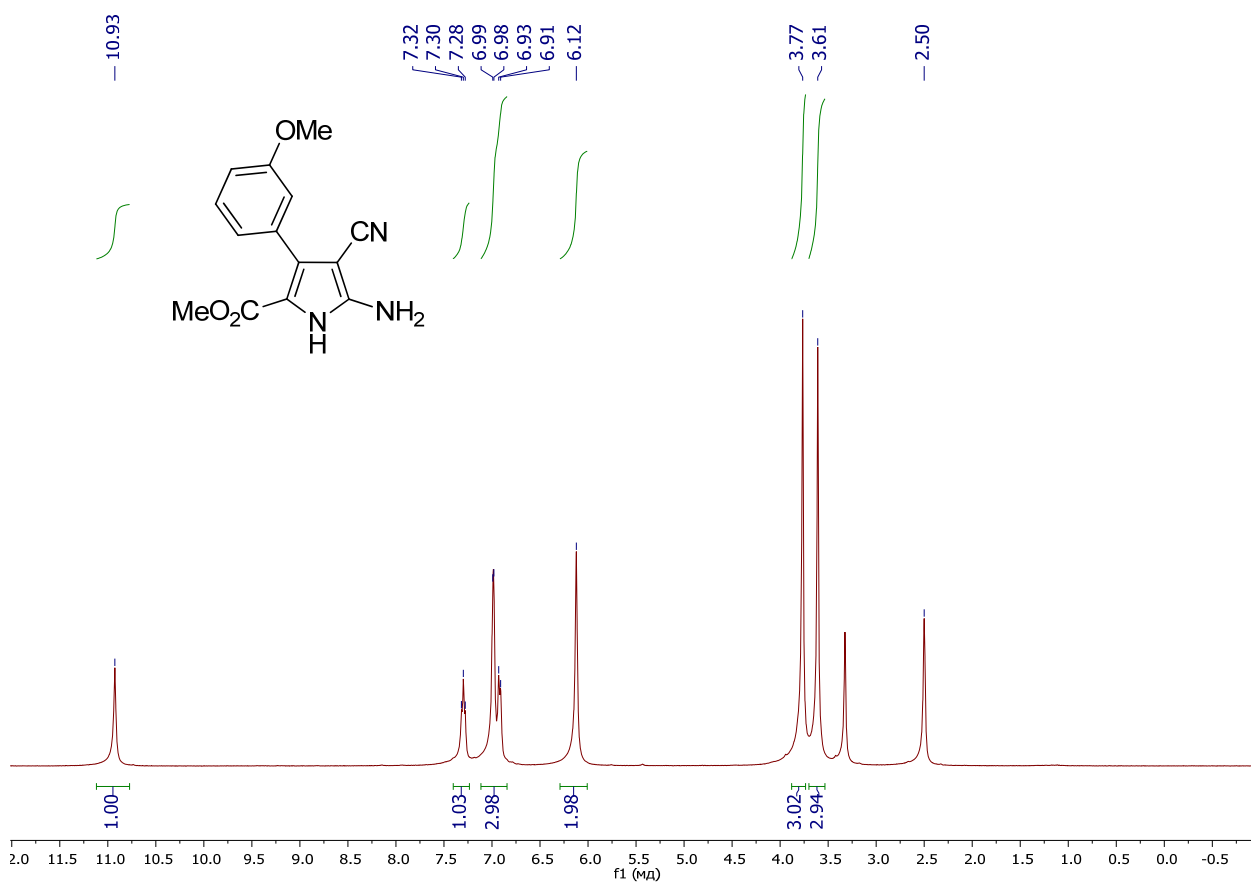f1 (мд)

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2e

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2e

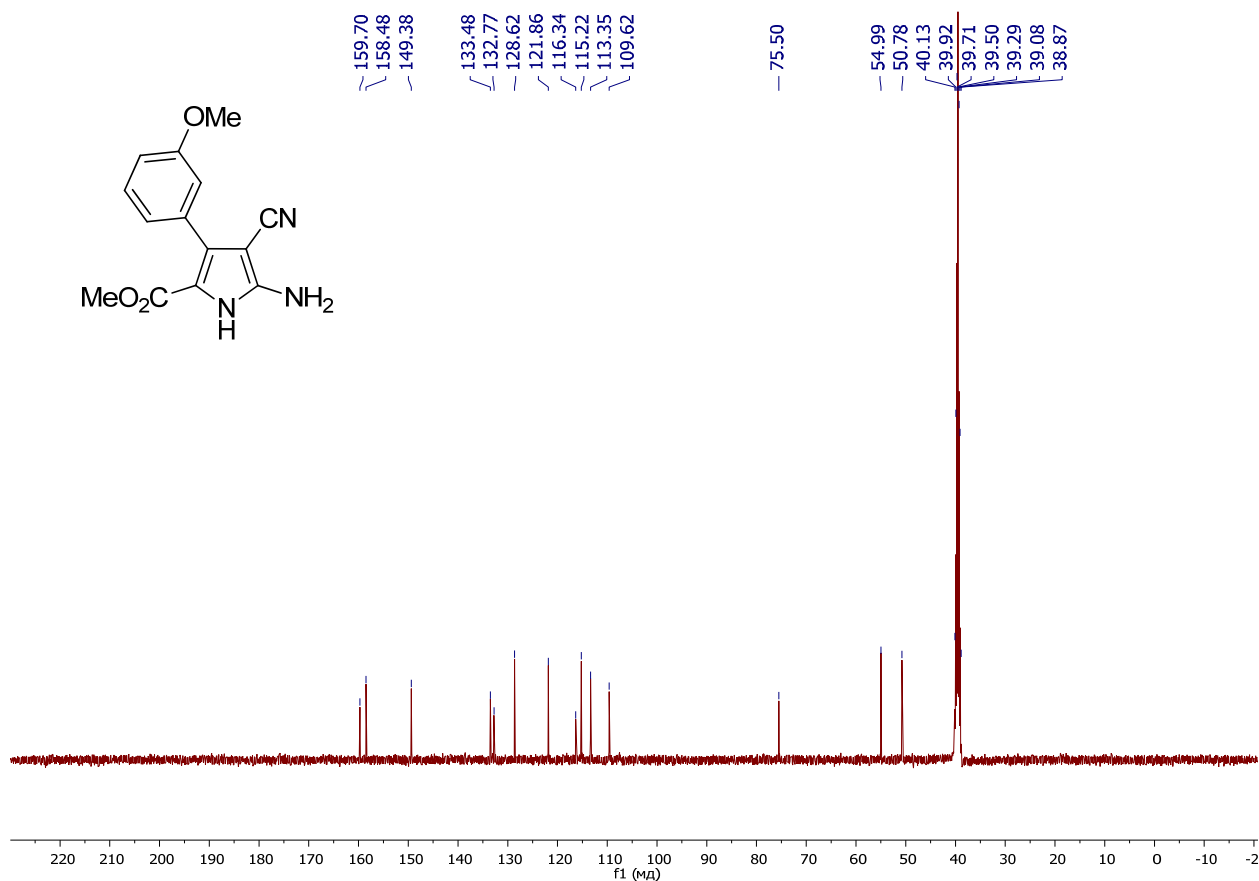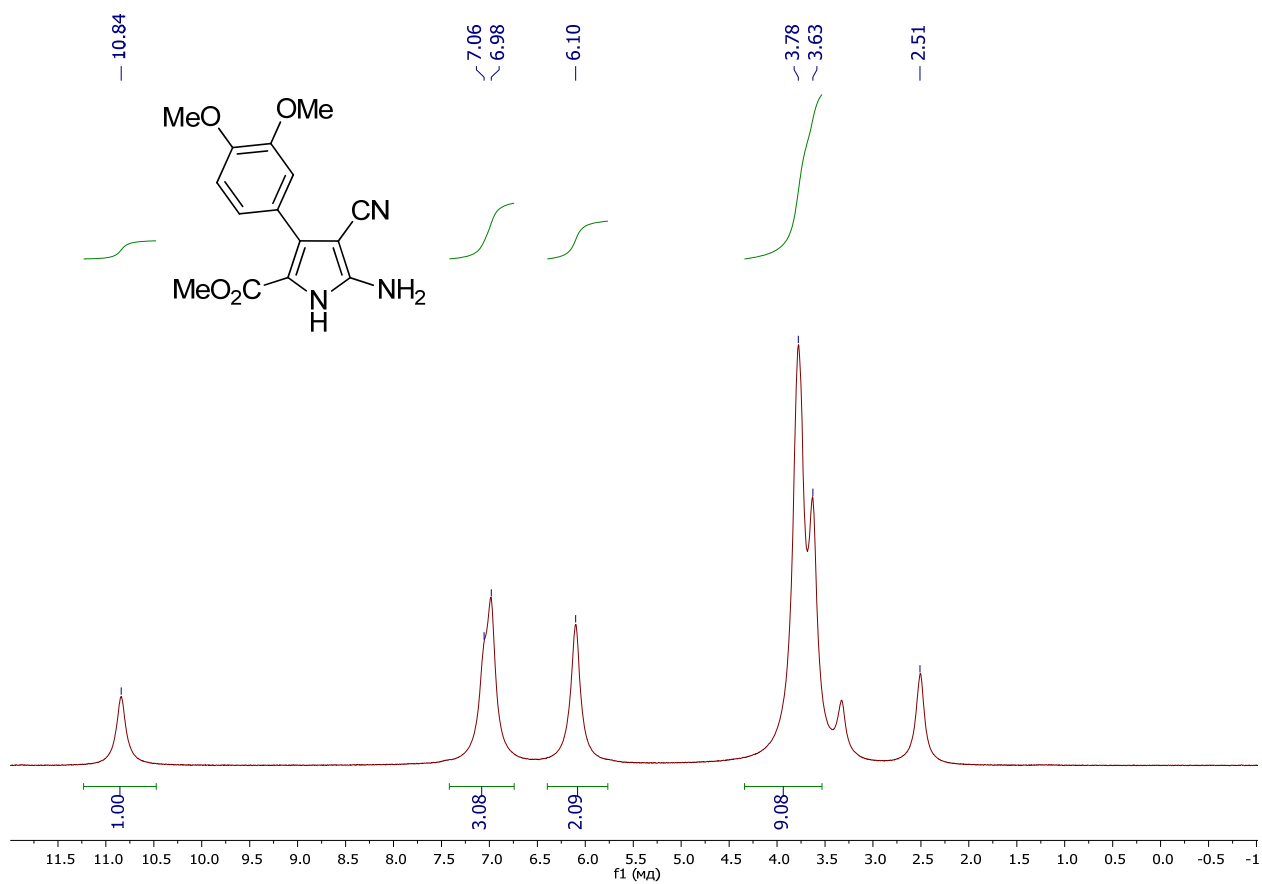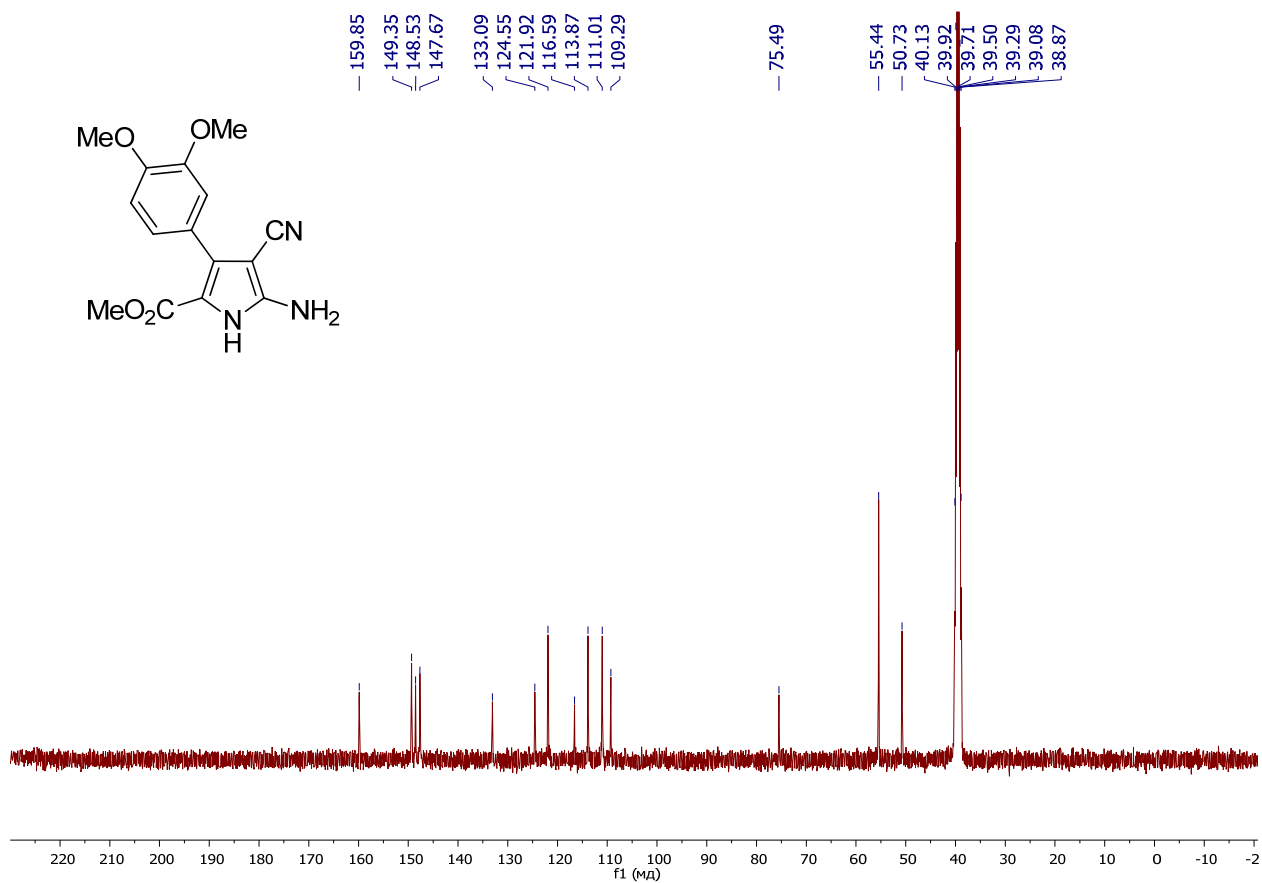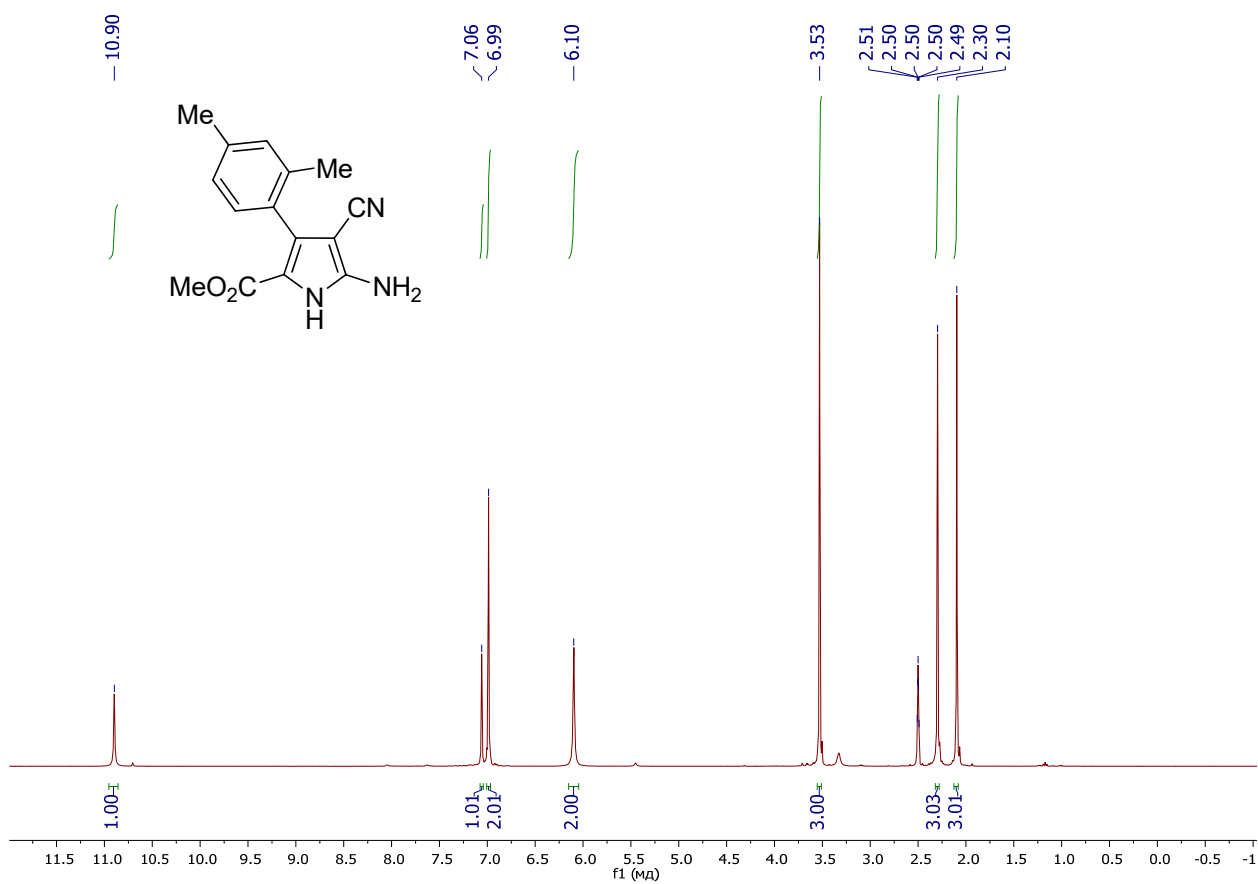## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2f**

10.84

7.06
6.98

6.10

3.78
3.63

2.51

MeO OMe

CN

MeO$_2$C NH$_2$

1.00

3.08

2.09

9.08

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2f**

159.85

149.35
148.53
147.67

133.09
124.55
121.92
116.59
113.87
111.01
109.29

75.49

55.44
50.73
40.13
39.92
39.71
39.50
39.29
39.08
38.87

MeO OMe

CN

MeO$_2$C NH$_2$

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2g**

10.90

7.06
6.99

6.10

3.53

2.51
2.50
2.50
2.50
2.49
2.30
2.10

Me

Me

CN

MeO$_2$C

N
H

NH$_2$

1.00

1.01
2.01

2.00

3.00

3.03
3.01

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2g**

159.59

149.05

136.70
135.92
132.82
130.15
129.75
125.74
116.20
110.42

76.42

50.70
40.13
39.92
39.71
39.50
39.29
39.08
38.88
20.71
19.35

Me

Me

CN

MeO$_2$C

N
H

NH$_2$

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S14

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2h**

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2h**

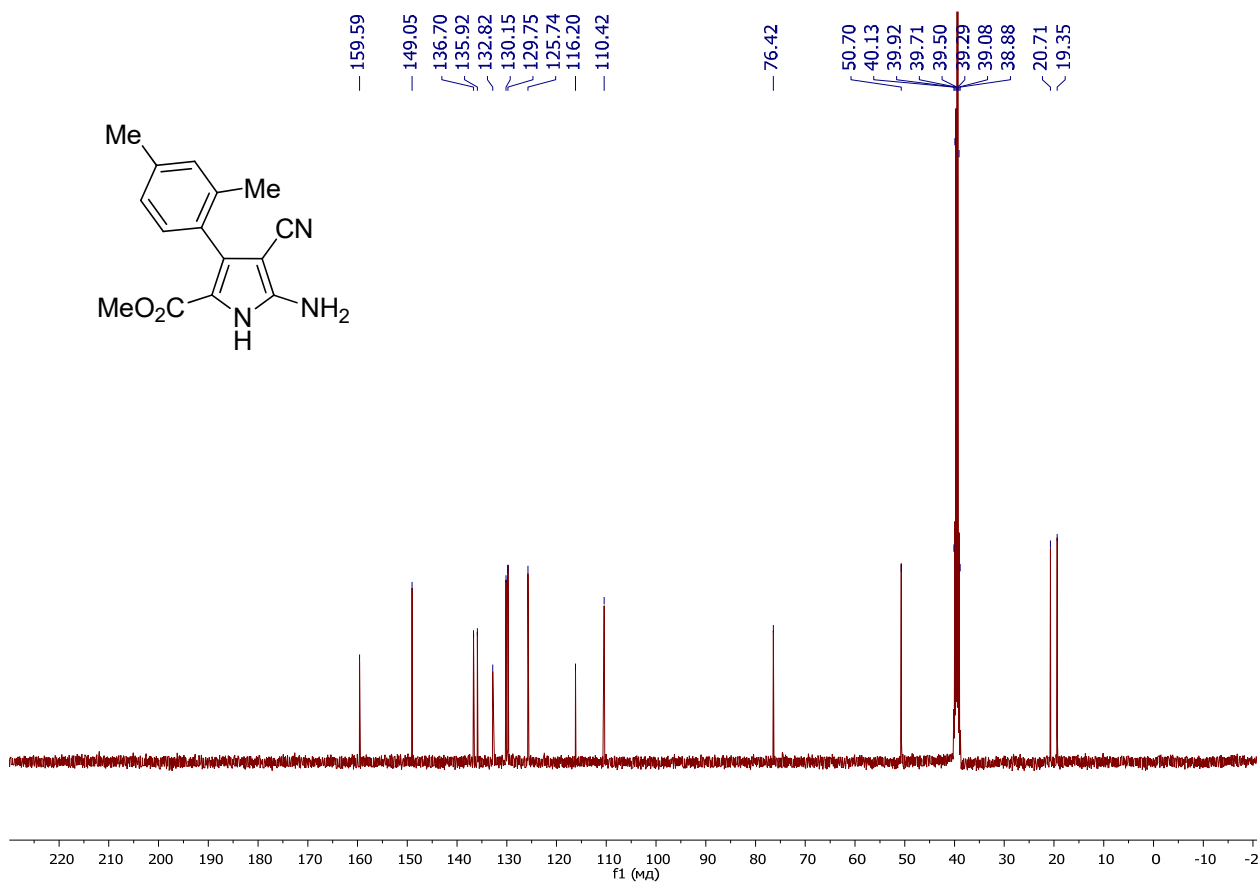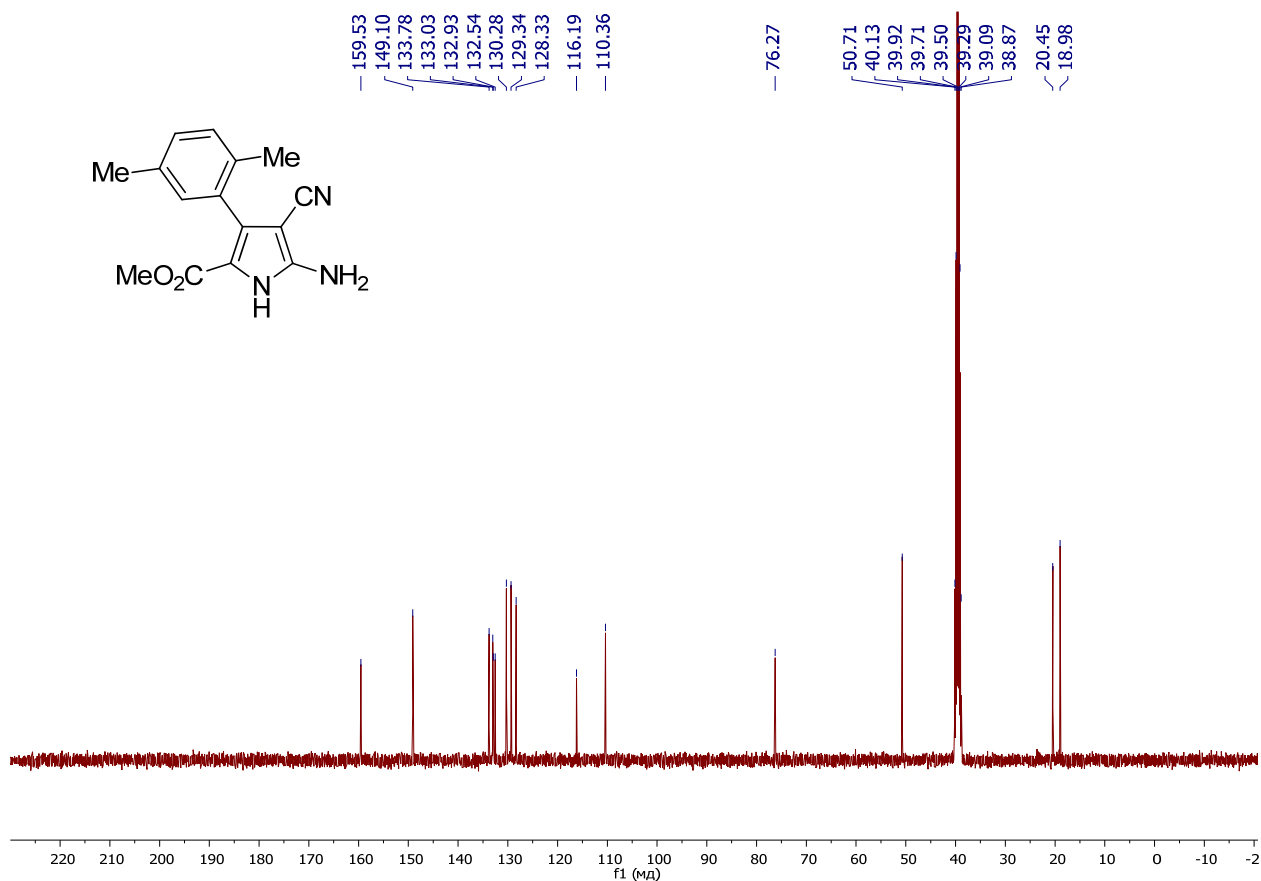# ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2i

11.20

8.26
8.24
7.70
7.68

6.25

3.62

2.50

1.00

2.11
2.06

2.00

3.05

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2i

159.44

149.67
146.69
139.26
130.88
130.30
122.79
115.88
110.49

75.08

51.00
40.13
39.92
39.71
39.50
39.29
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
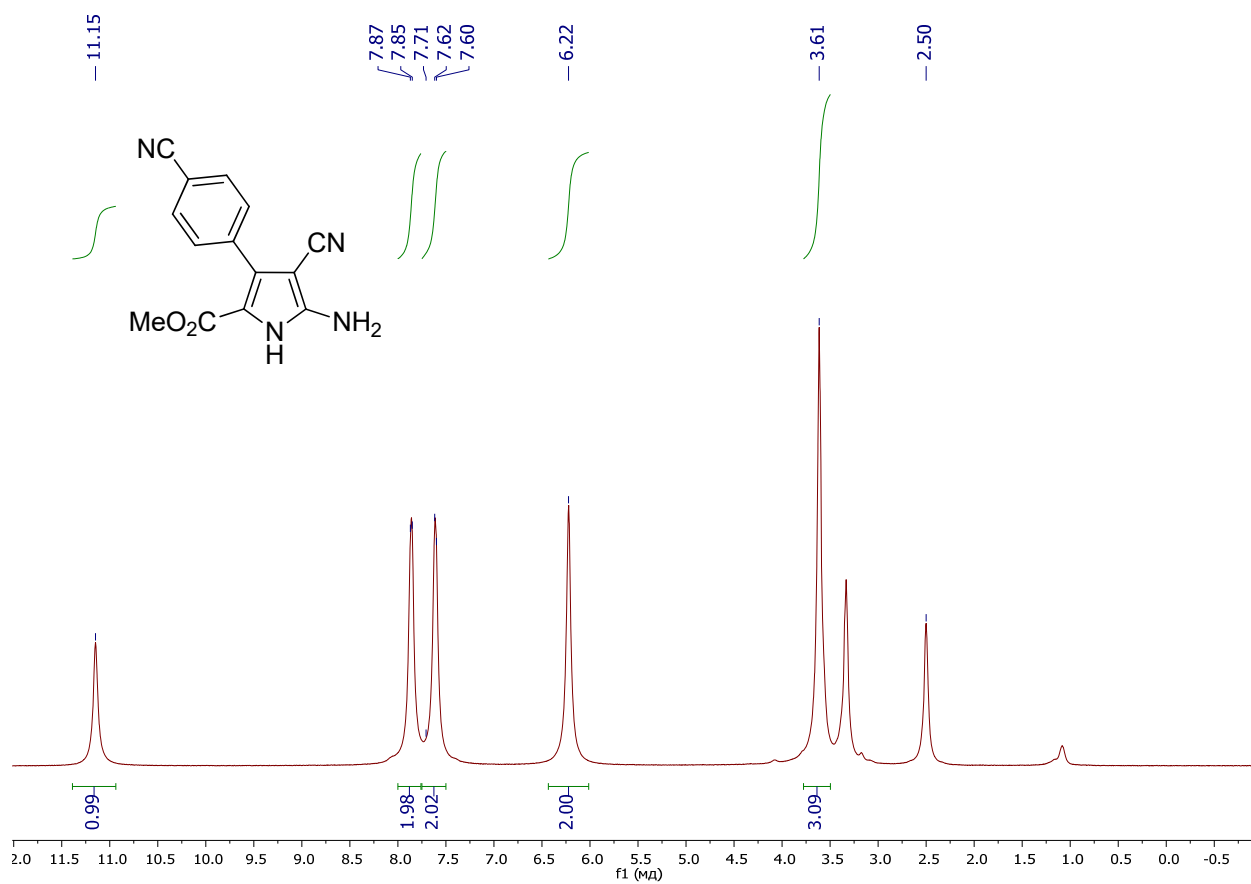f1 (мд)

S16
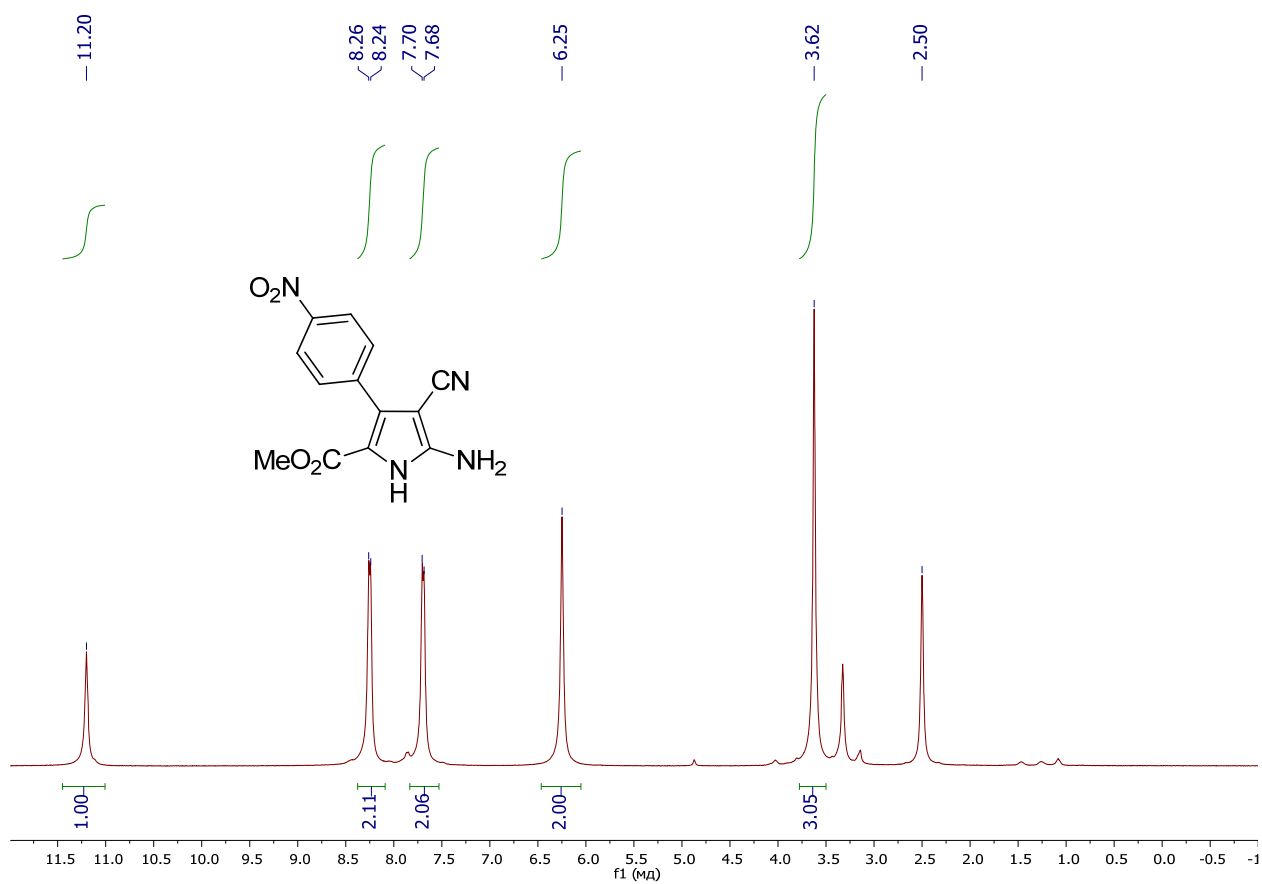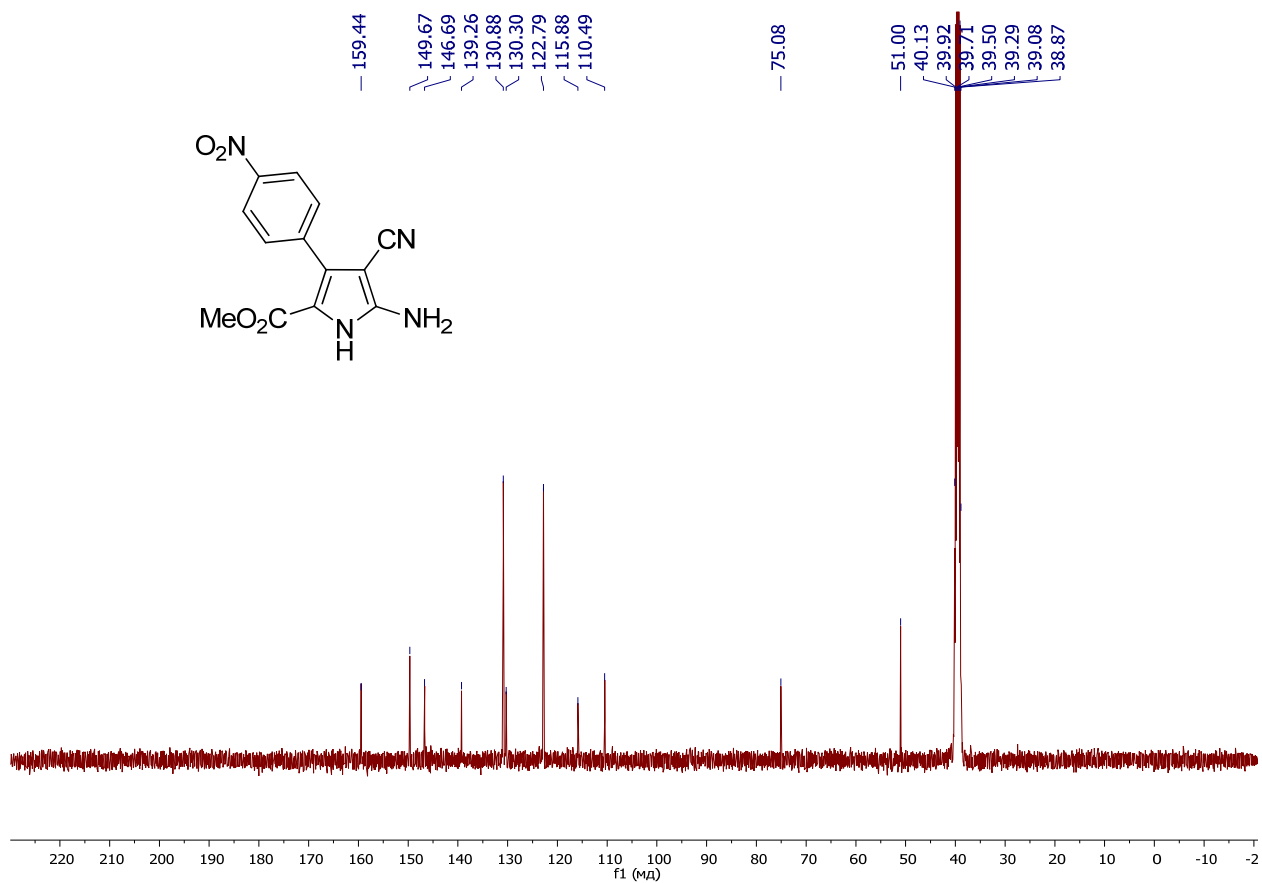
^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2j

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2j
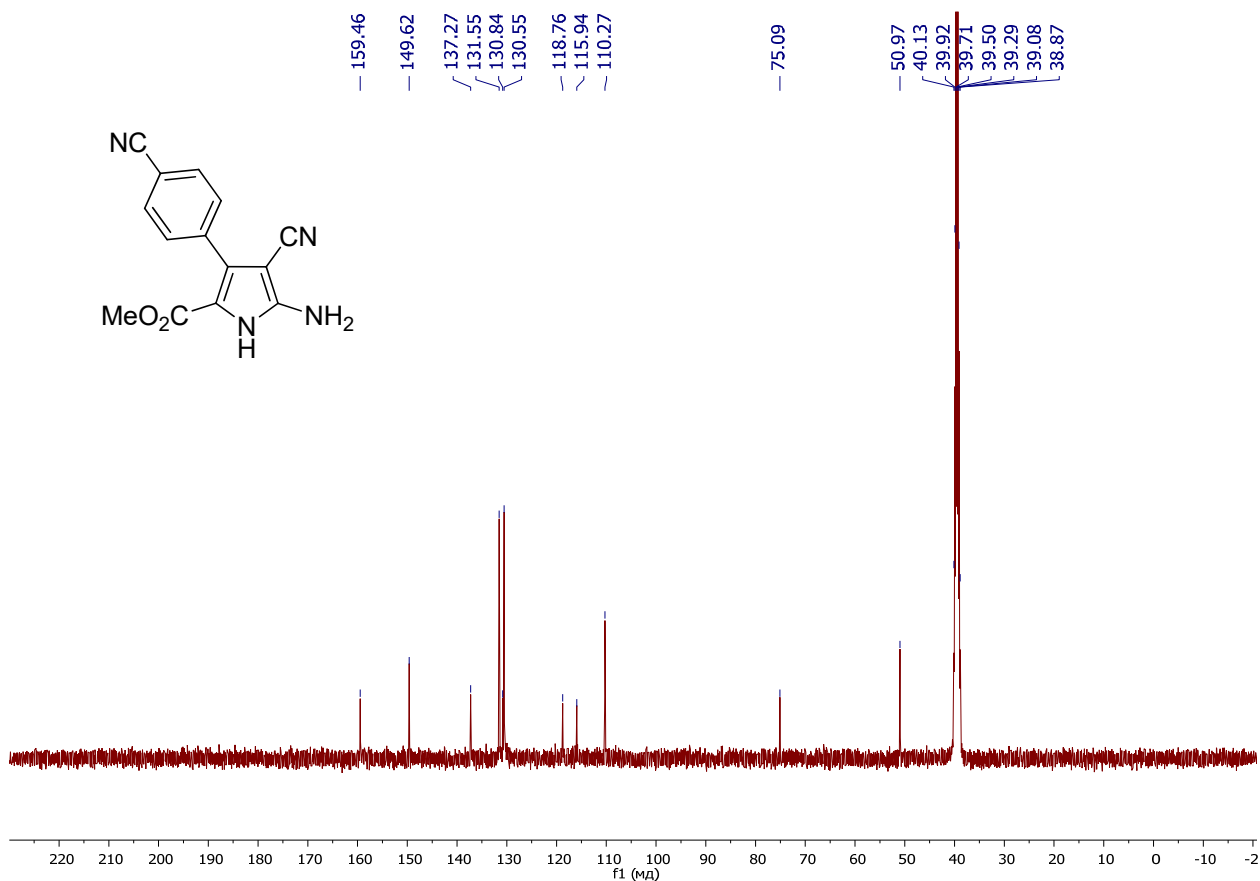
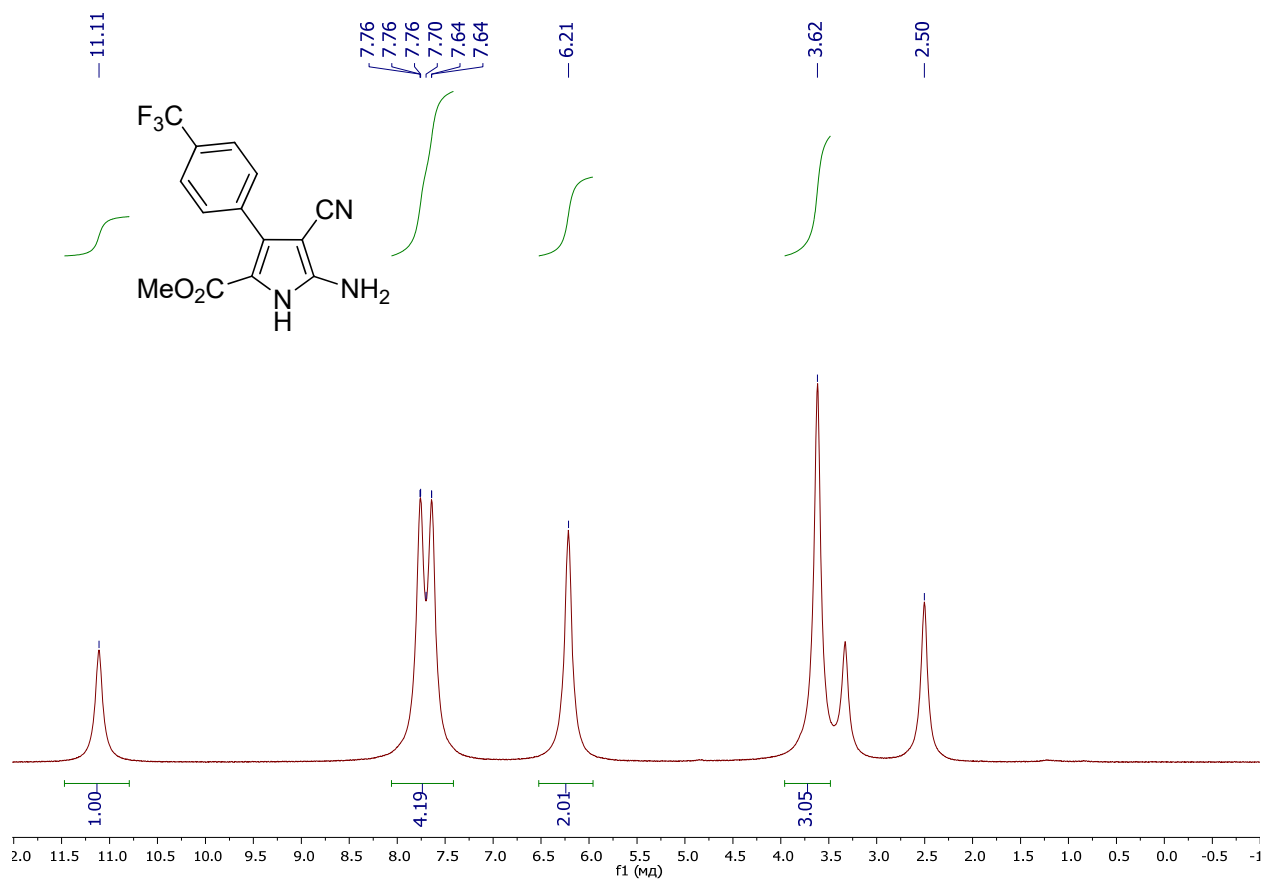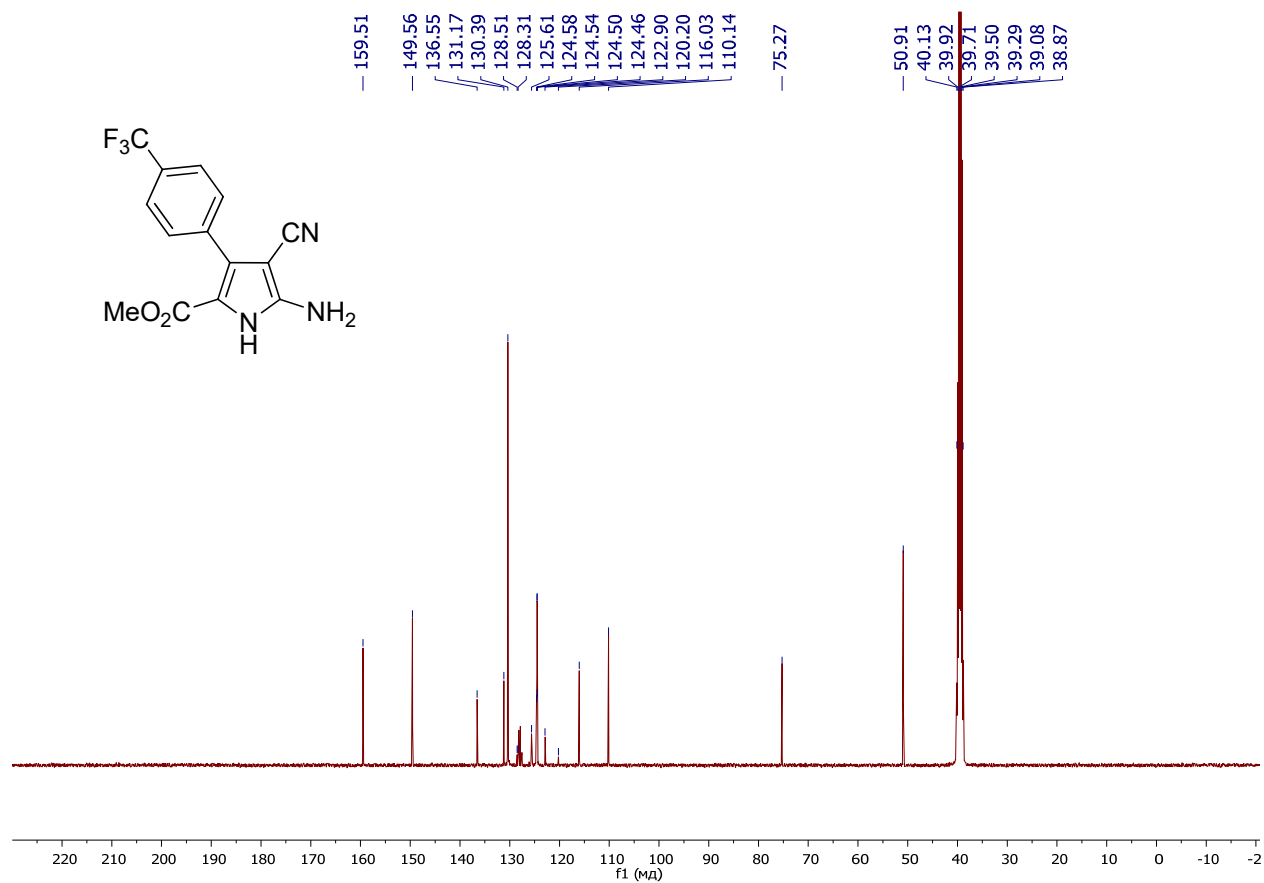## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2k

11.11
7.76
7.76
7.76
7.70
7.64
7.64
6.21
3.62
2.50

1.00
4.19
2.01
3.05

2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2k

159.51
149.56
136.55
131.17
130.39
128.51
128.31
125.61
124.58
124.54
124.50
124.46
122.90
120.20
116.03
110.14
75.27
50.91
40.13
39.92
39.71
39.50
39.29
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S18

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2l

10.96

7.47 7.45 7.45 7.43 7.24 7.22 7.20

6.15

3.60

2.50

0.95

2.02 2.00

2.04

3.03

f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2l

162.93 160.50 159.64

149.37

131.97 131.66 131.57 128.61 128.57 116.25 114.64 114.43 109.70

75.48

50.80 40.13 39.92 39.71 39.50 39.29 39.08 38.88

f1 (мд)

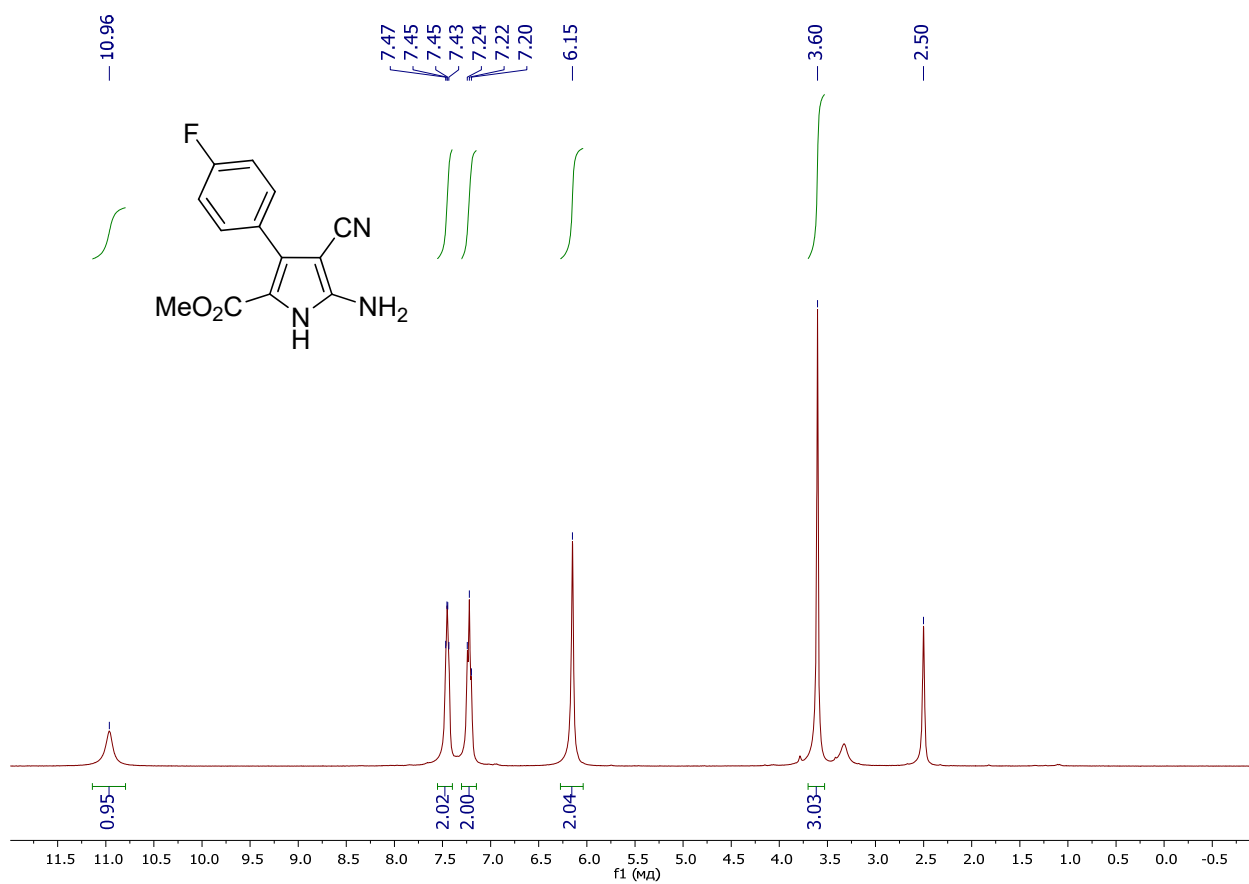¹H NMR spectra (DMSO-*d*₆, 400 MHz) of compound **2m**

¹³C NMR spectra (DMSO-*d*₆, 100 MHz) of compound **2m**

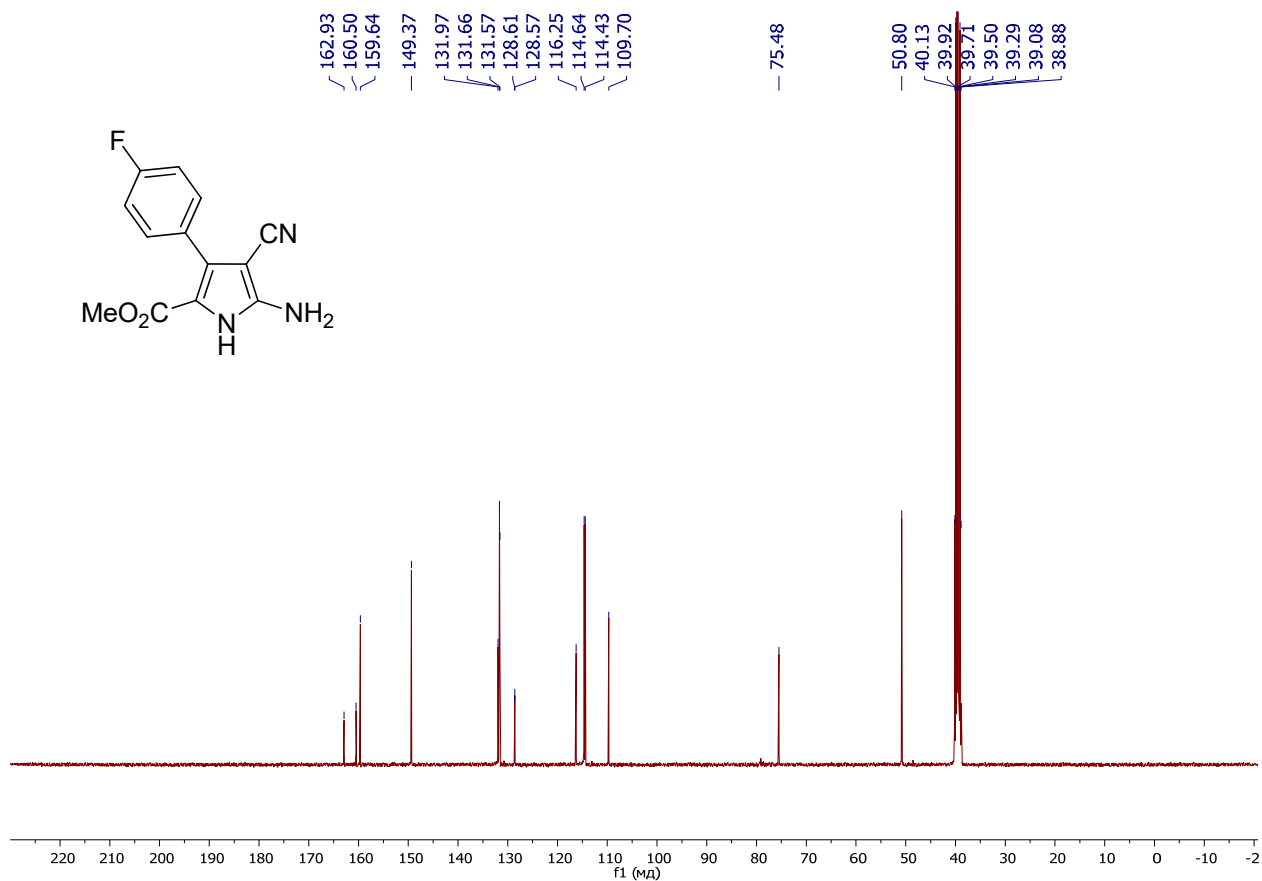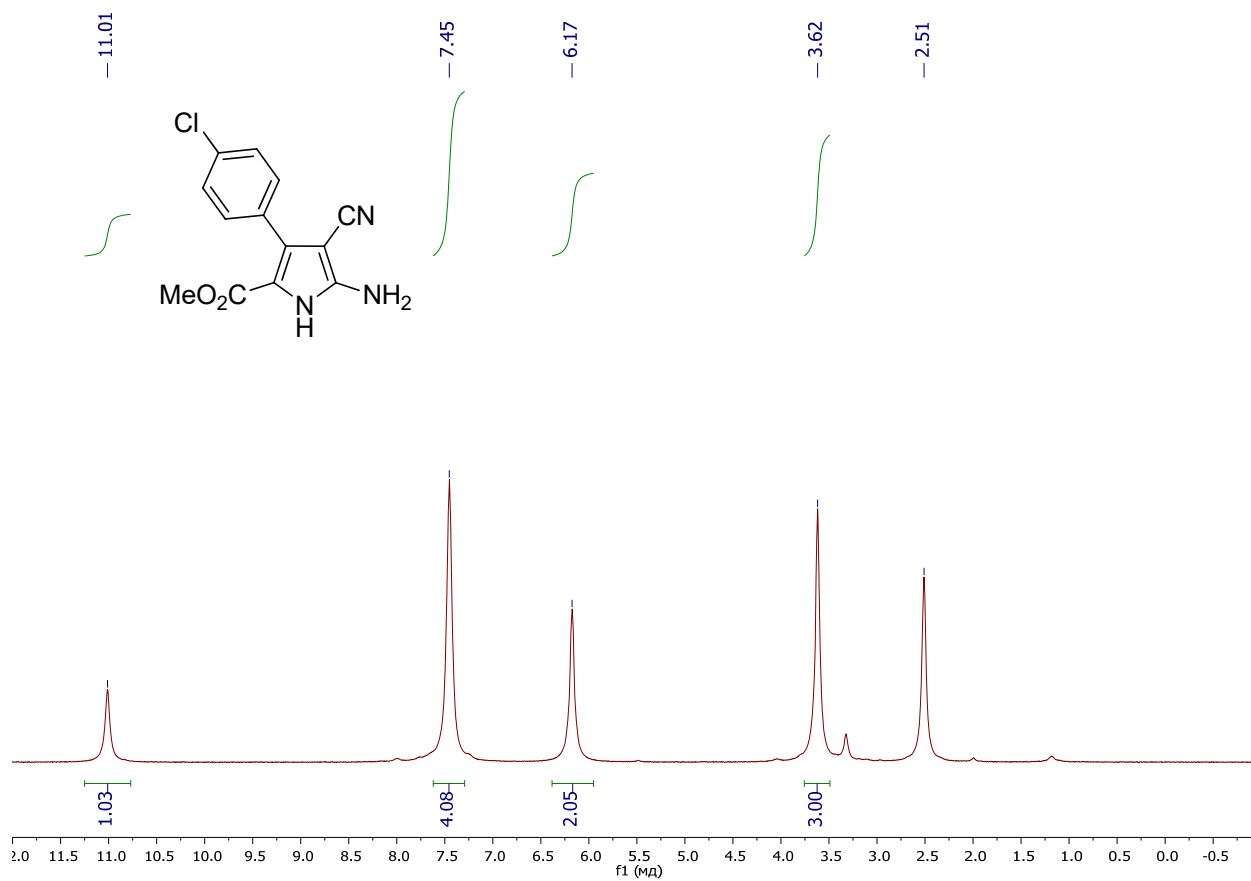## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2n**

7.60
7.58
7.37
7.35
11.01
6.17
3.61
2.50

0.98
2.11
2.11
2.00
3.08

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2n**

159.58
149.44
131.63
131.59
131.50
130.60
121.06
116.13
109.73
75.22
50.84
40.13
39.92
39.71
39.50
39.29
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

¹H NMR spectra (DMSO-d_6, 400 MHz) of compound **2o**

¹³C NMR spectra (DMSO-d_6, 100 MHz) of compound **2o**

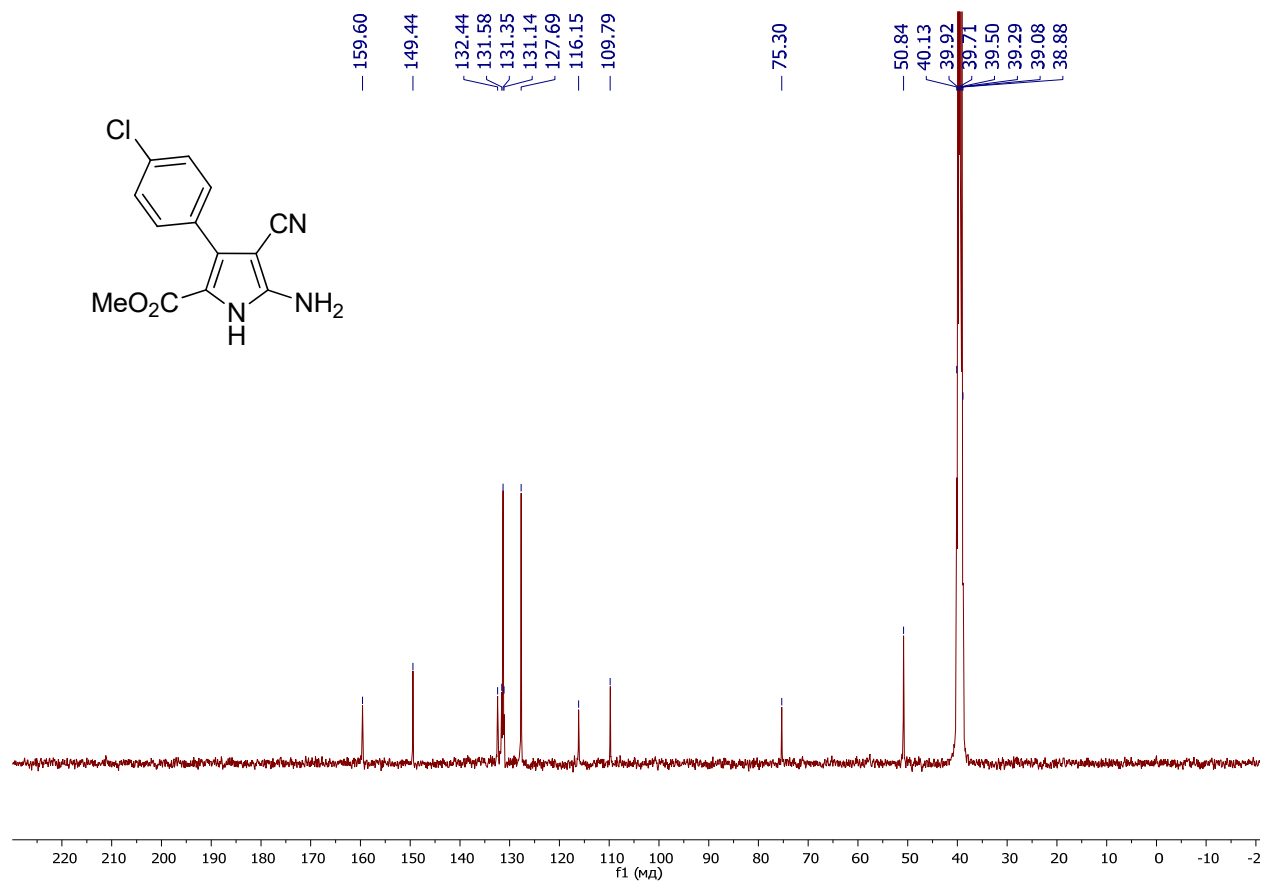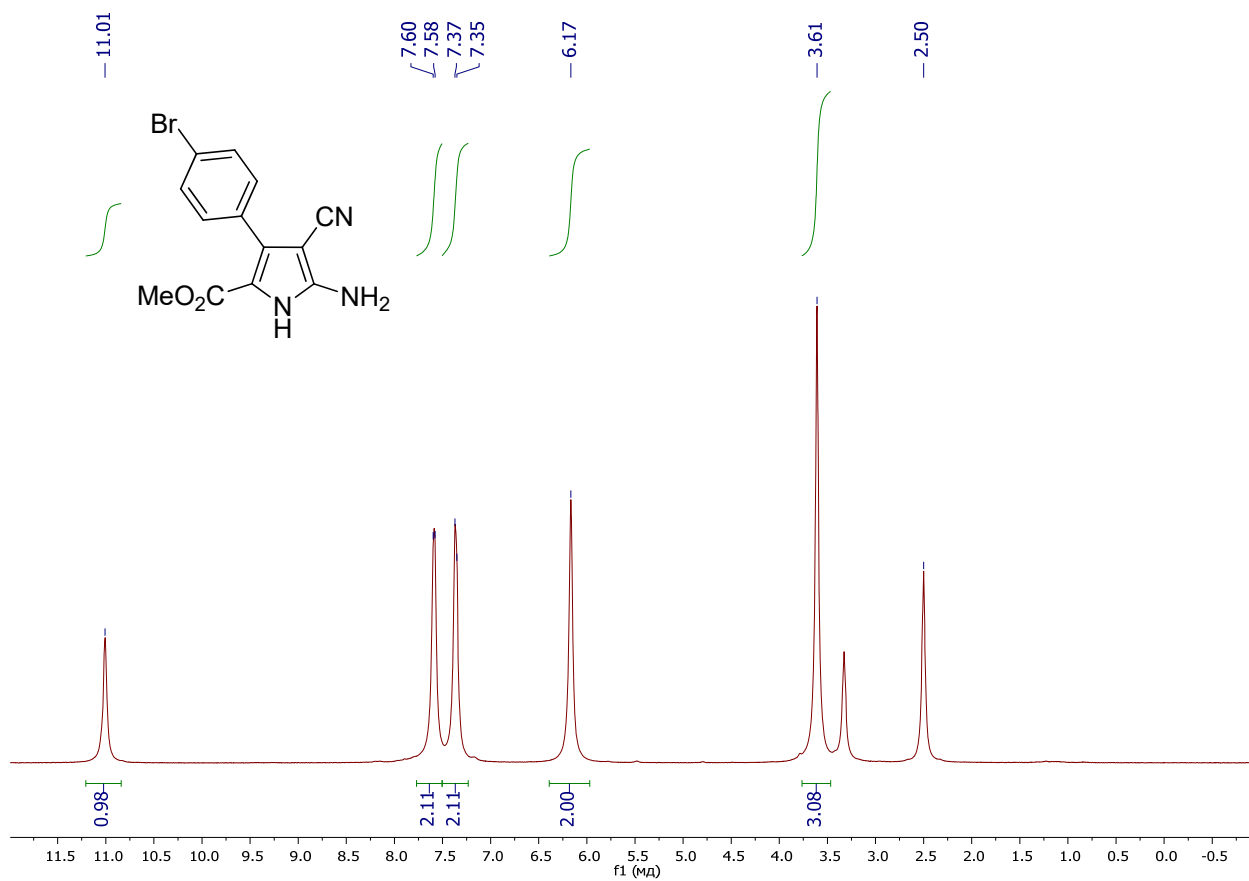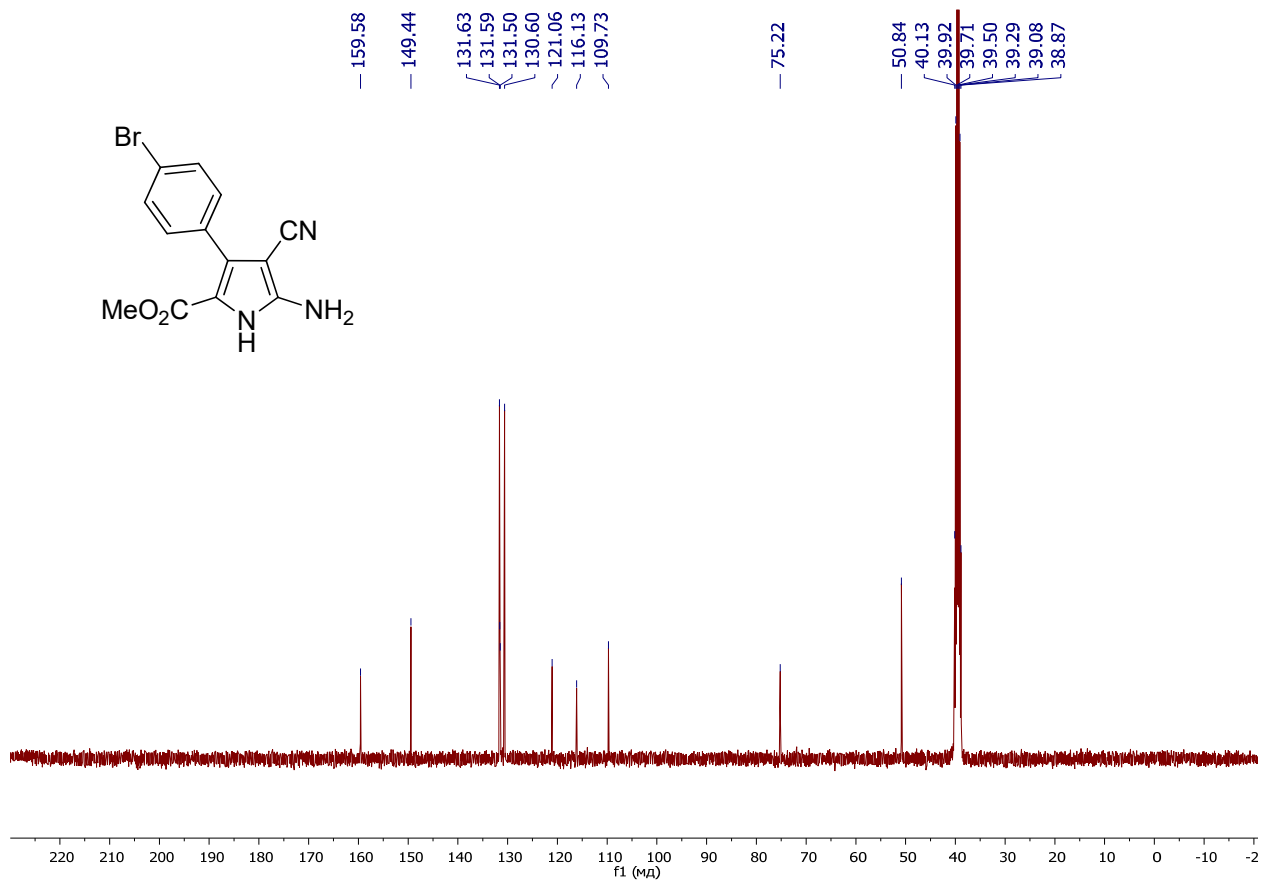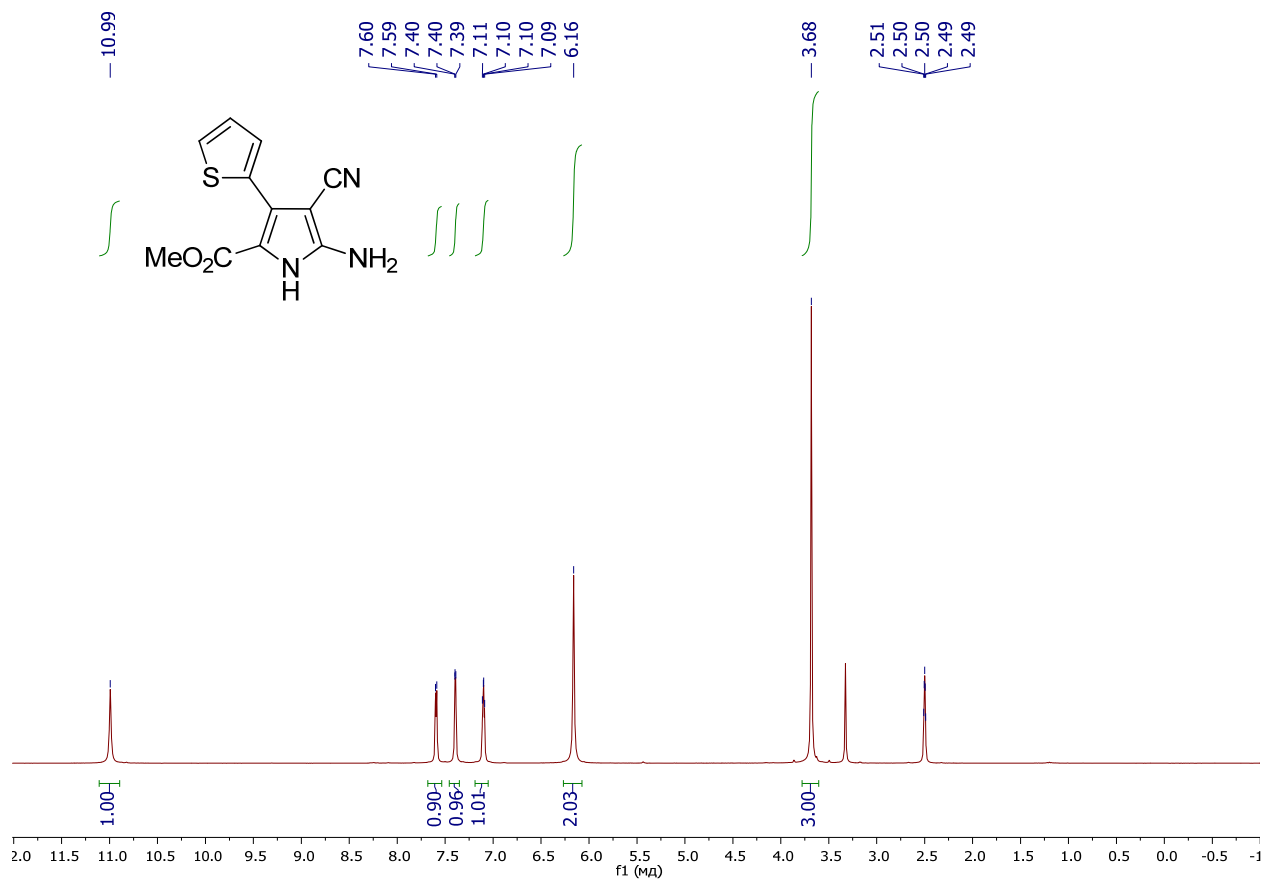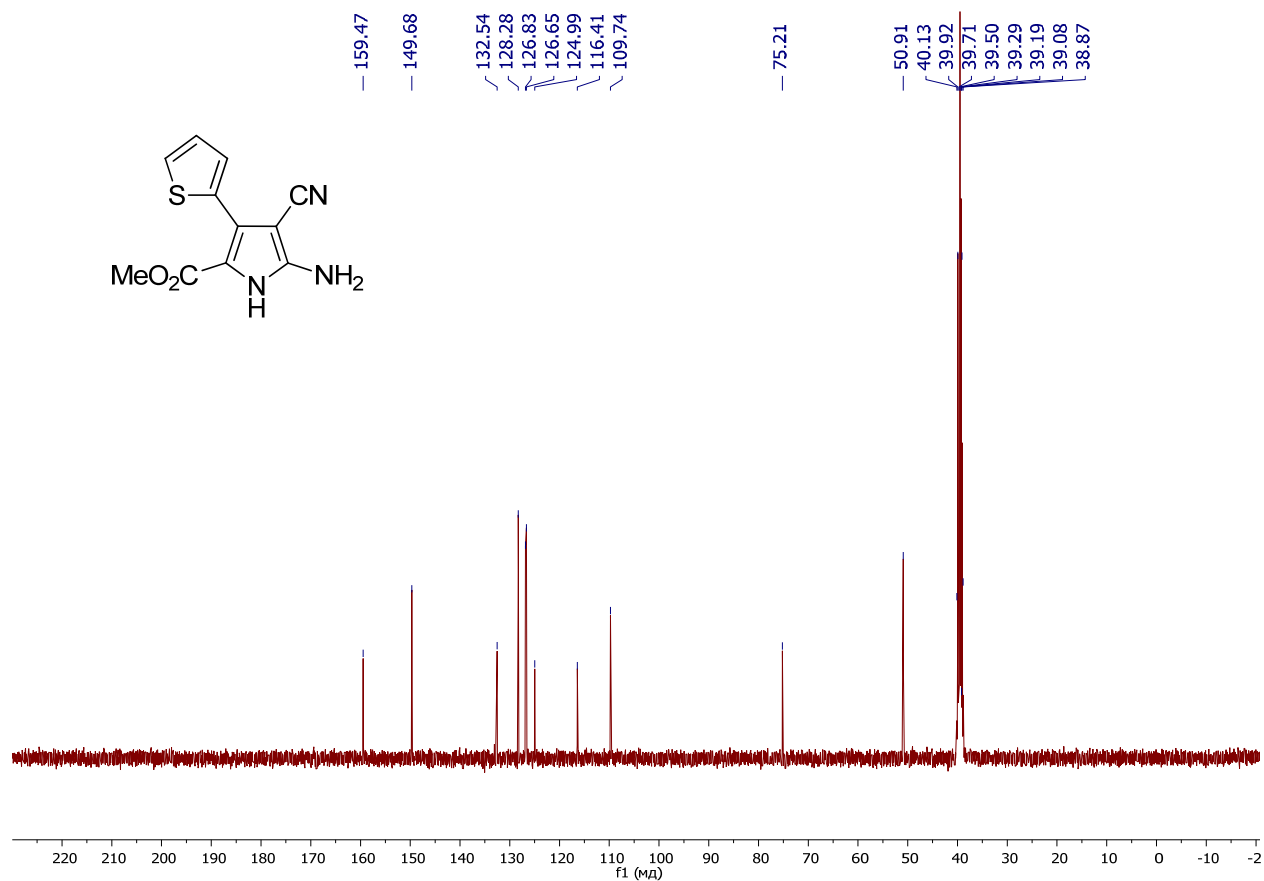# ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2p**

10.57

6.02

3.70

2.51
2.51
2.50
2.50
2.49
2.21

Me   CN

MeO$_2$C   NH$_2$
        N
        H

0.94   1.91   3.05   3.00

2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2p**

160.17

148.81

130.34

116.16
110.28

76.13

50.67

40.18
40.12
39.92
39.71
39.50
39.29
39.08
38.87
11.23

Me   CN

MeO$_2$C   NH$_2$
        N
        H

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S23

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2q**

10.89

7.42 7.41 7.40 7.39 7.38 7.36 7.35 7.35 7.34 7.33 7.31 7.29 7.28 7.27 7.21 7.20 7.19 7.18

6.18

5.12

2.51 2.50 2.49

1.00

1.97 6.01 1.98

2.03

2.16

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2q**

159.08

149.50

136.11 133.59 132.27 129.59 128.22 127.75 127.64 127.61

116.27

109.55

75.75

64.90

40.13 39.92 39.71 39.50 39.29 39.08 38.87

165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20

f1 (мд)

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2r**
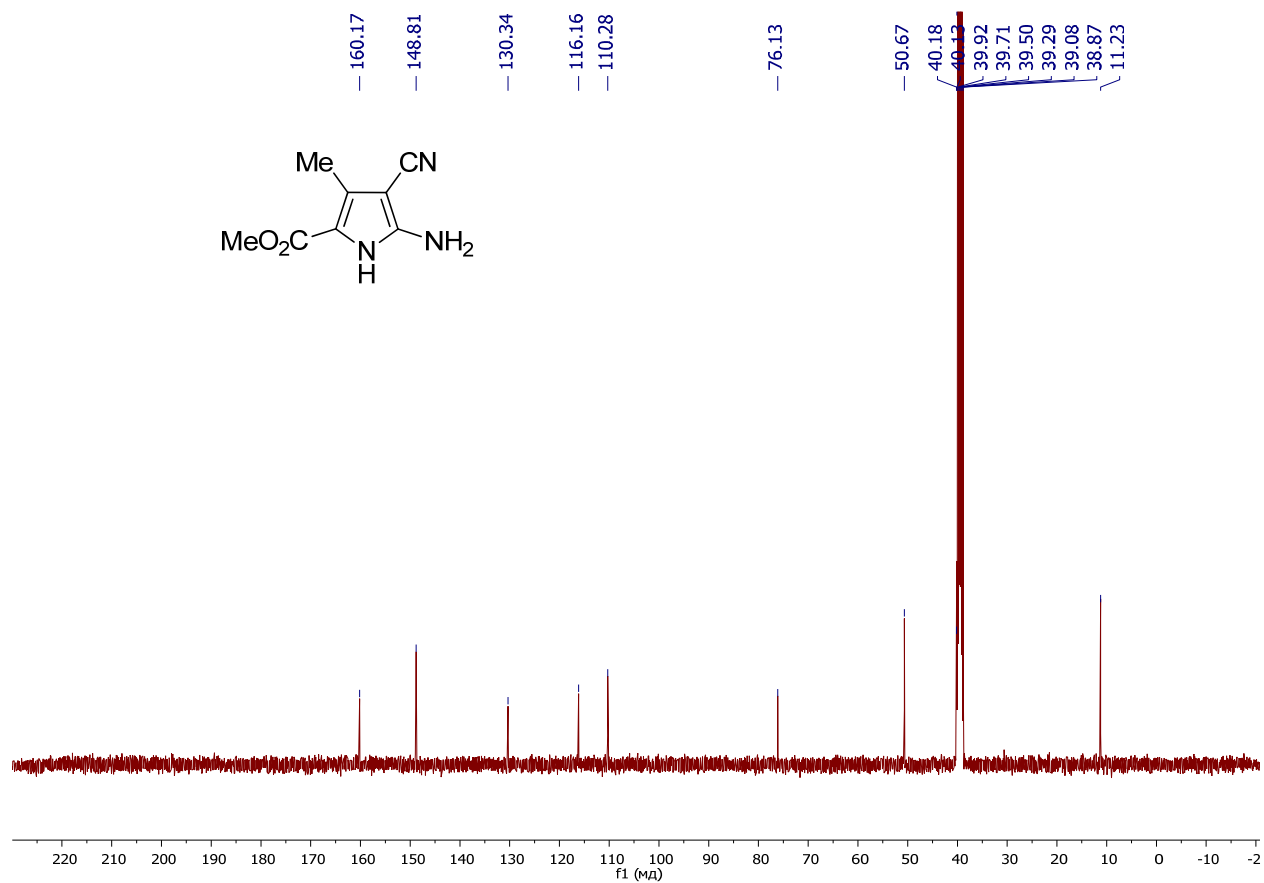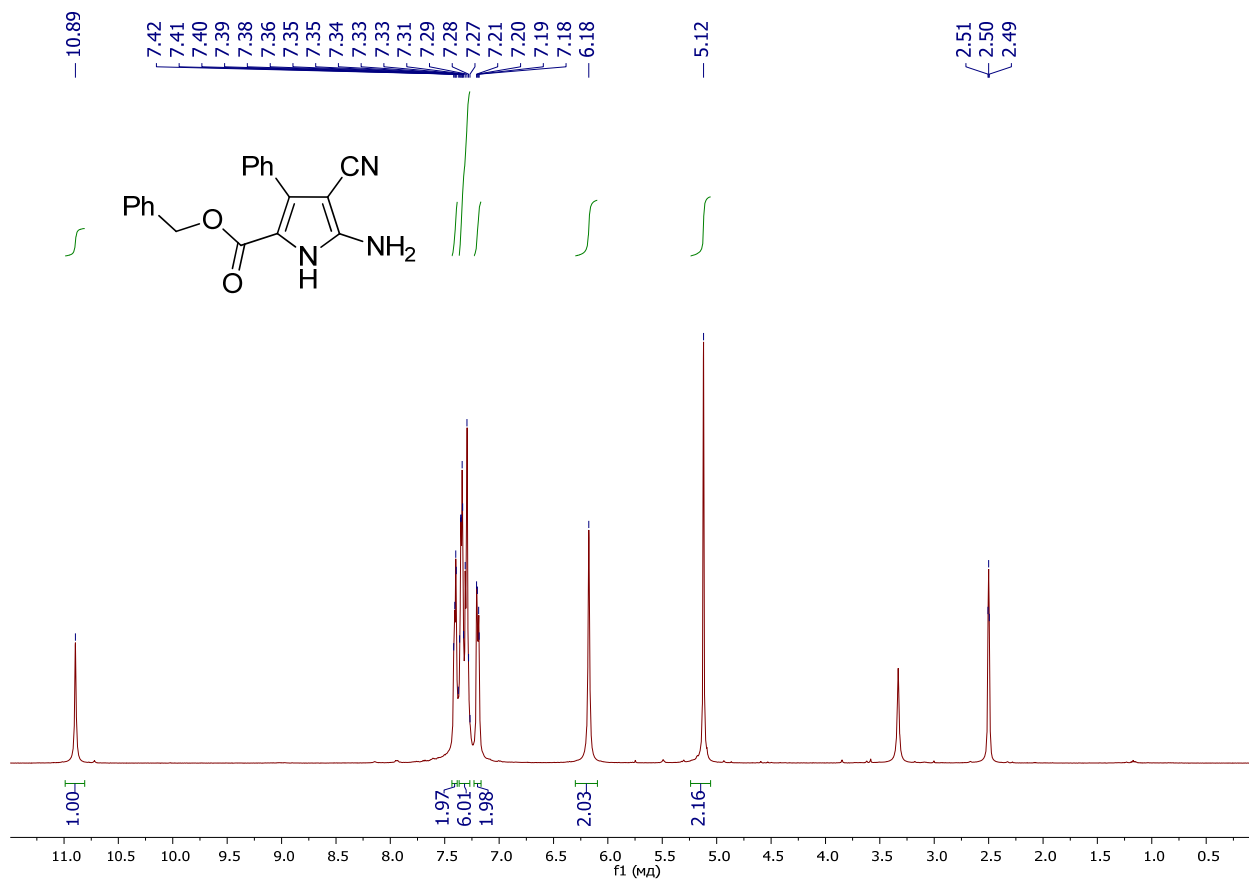

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2r**

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 2s

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 2s
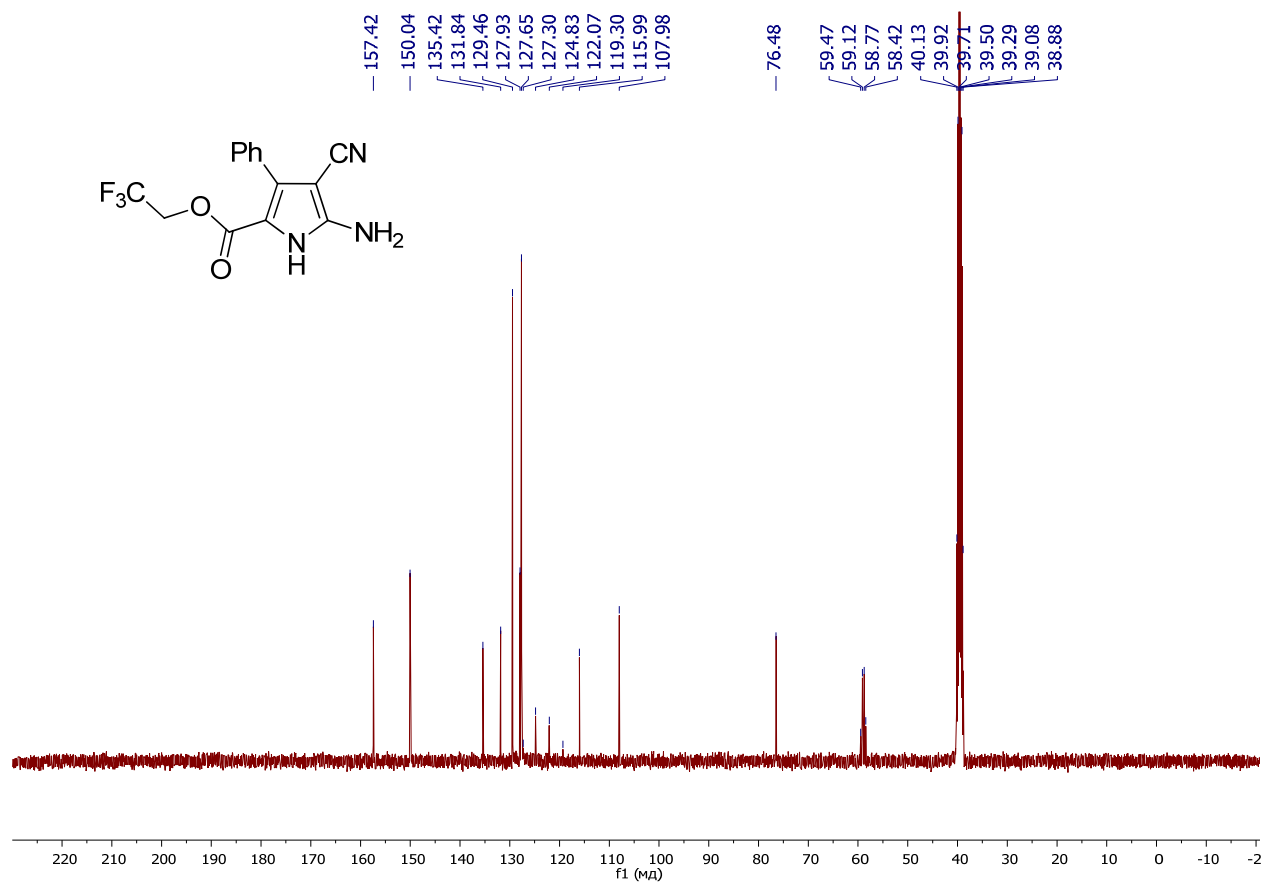
^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **2t**
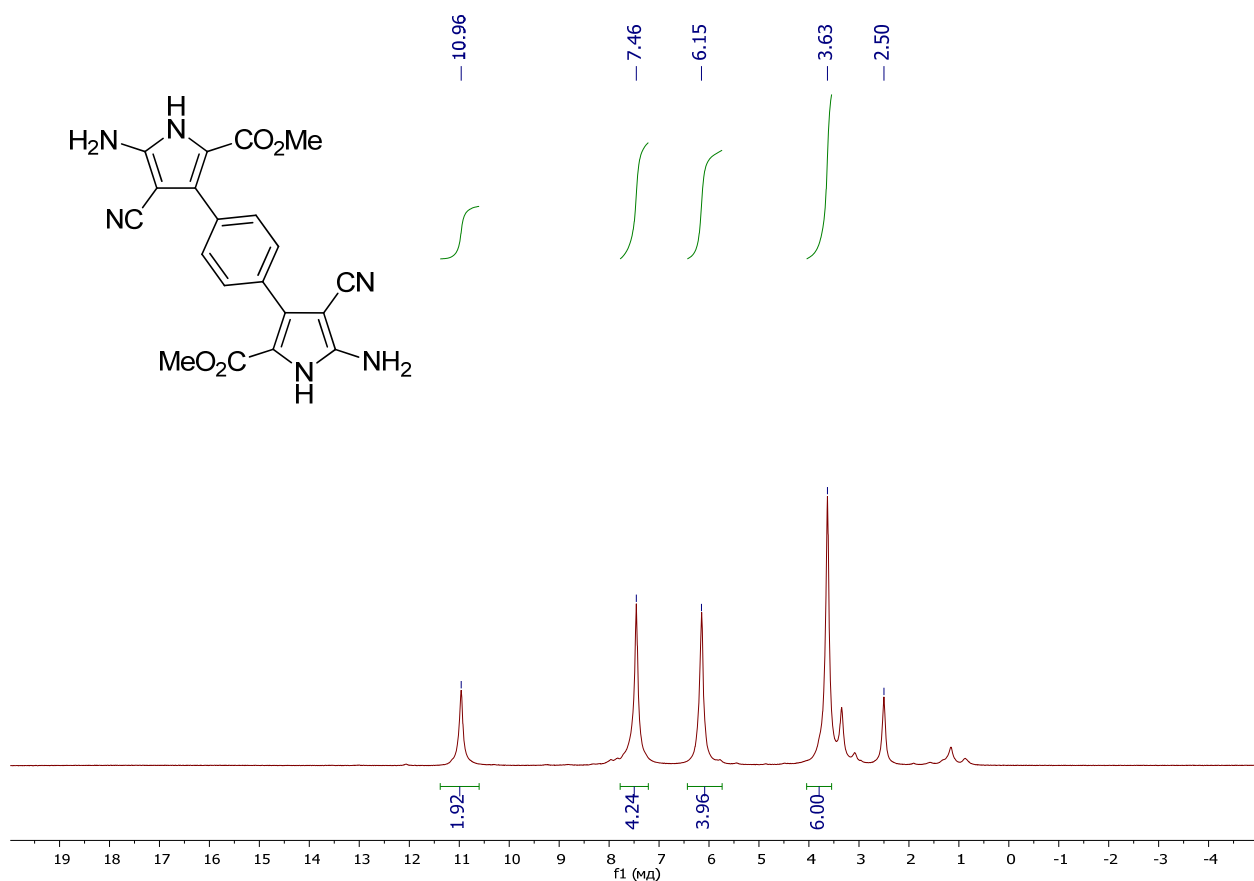
^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **2t**

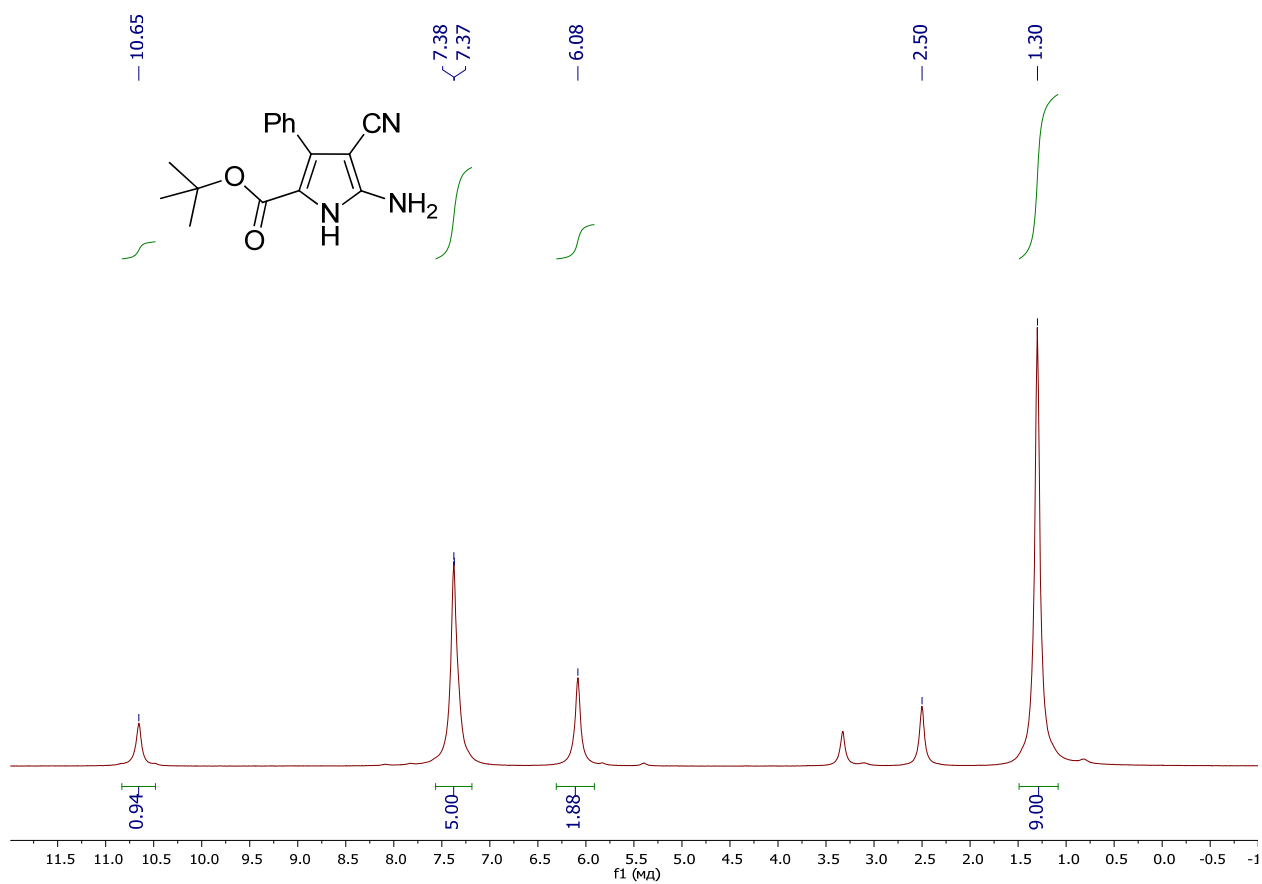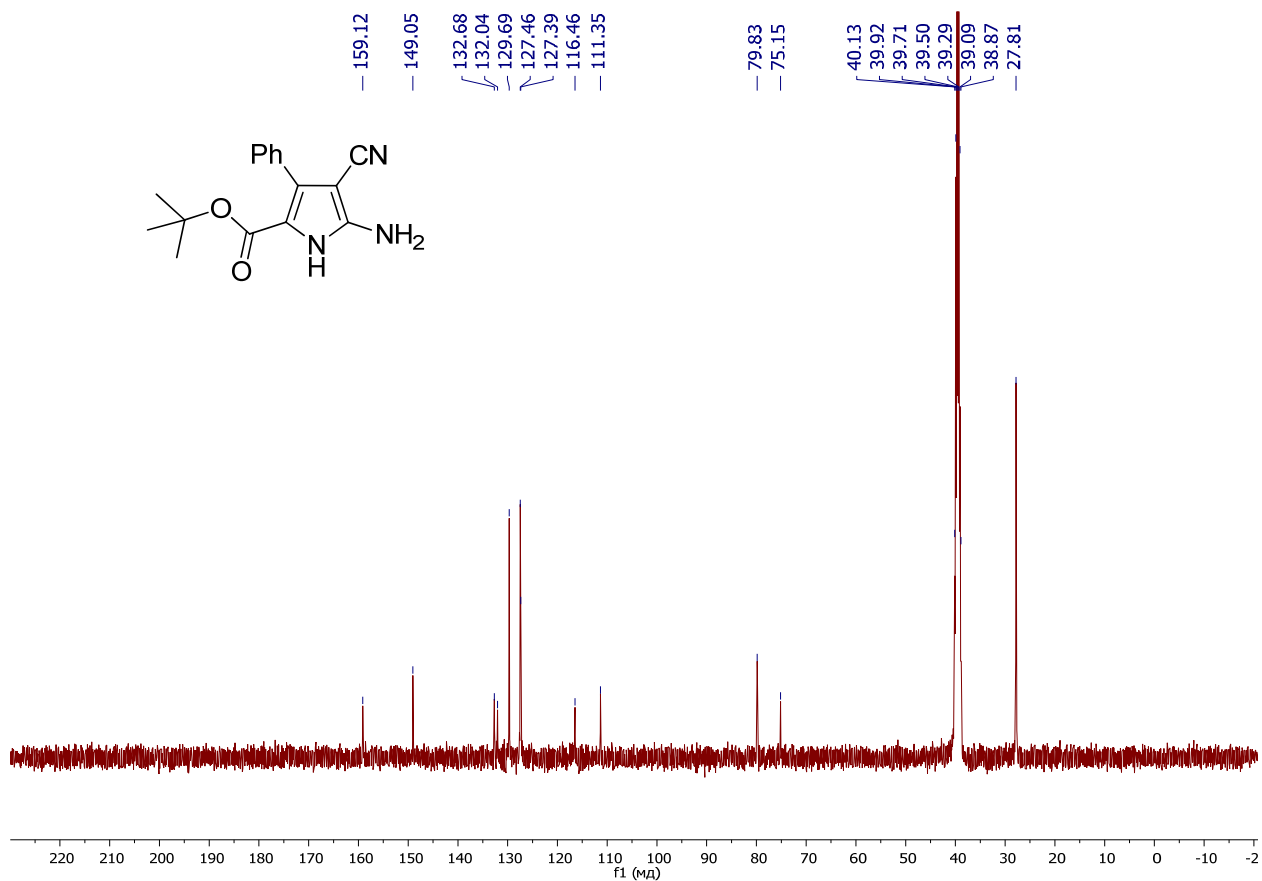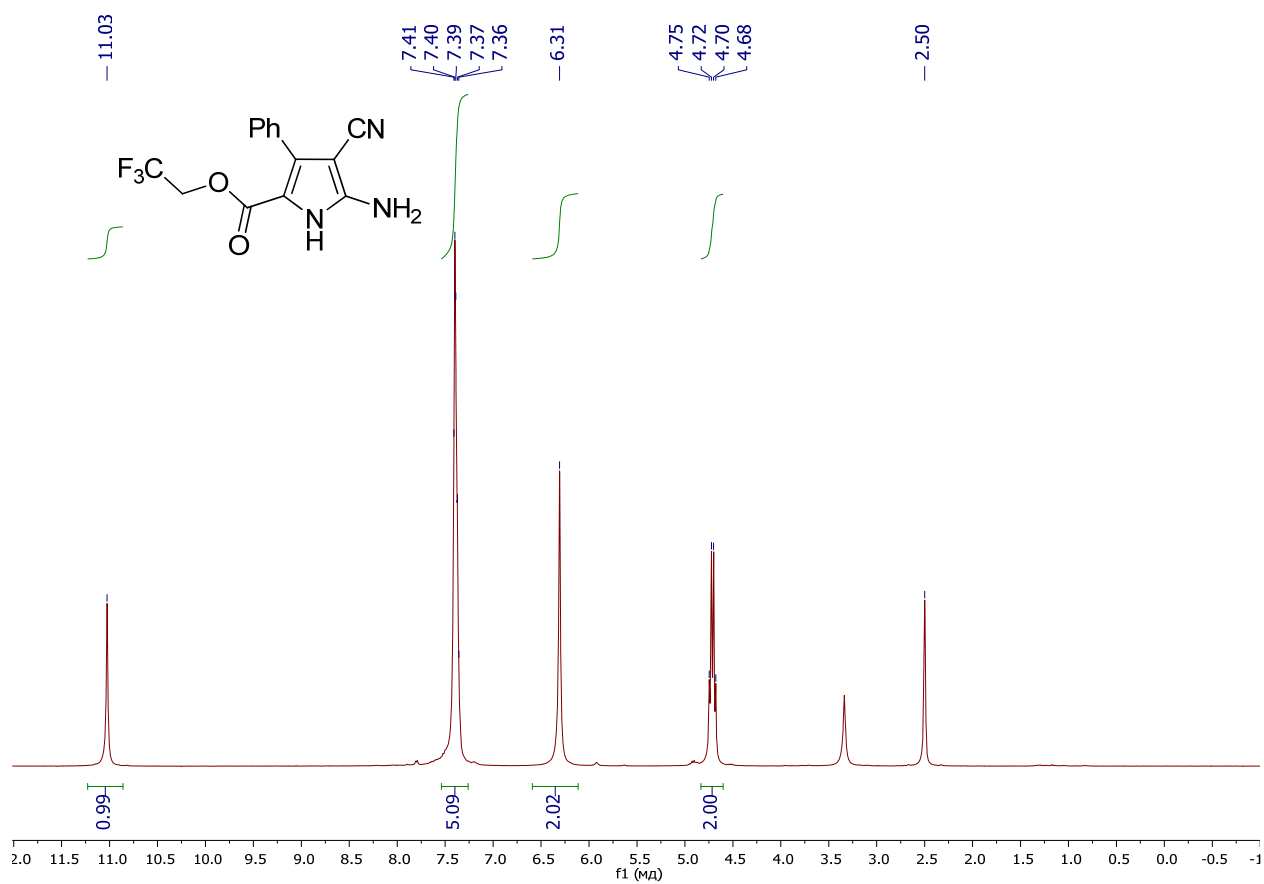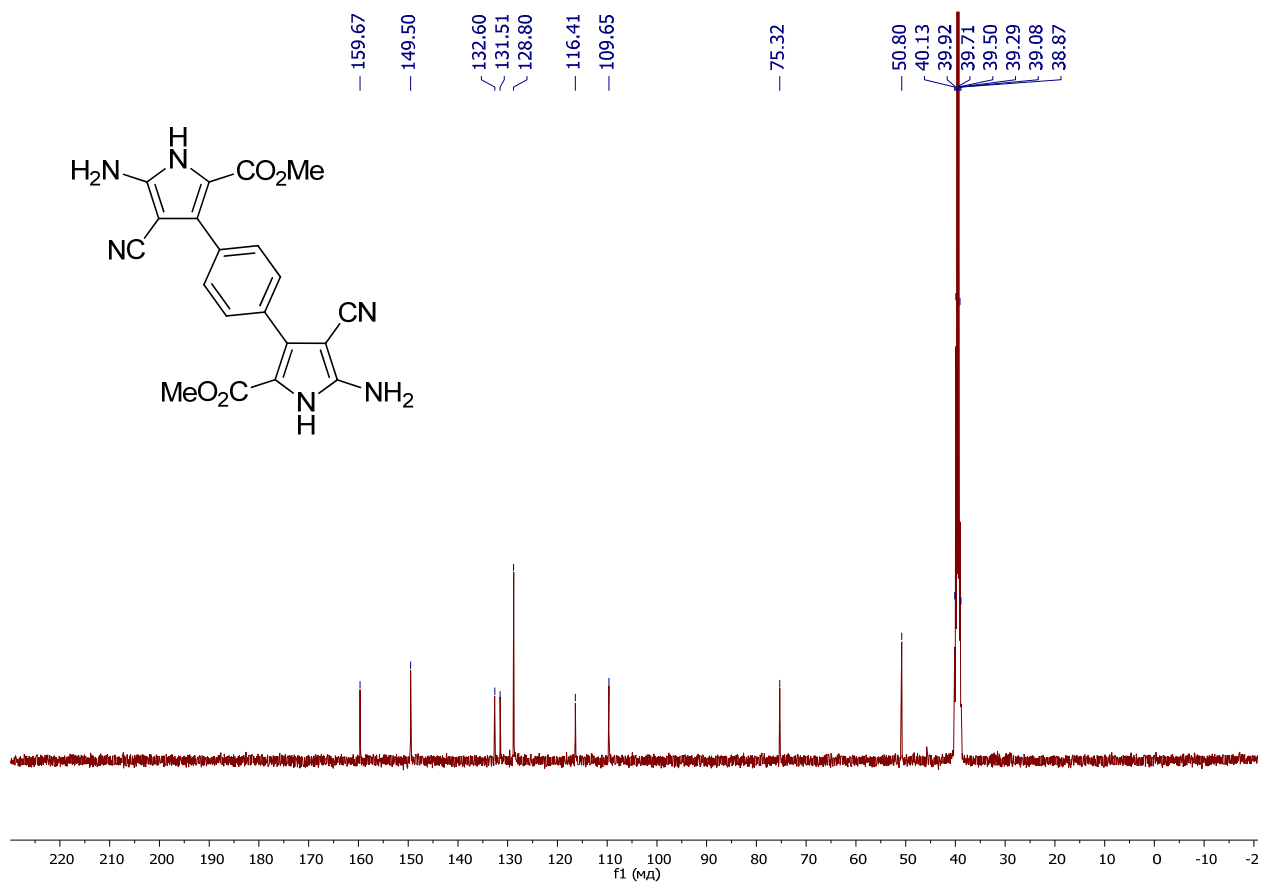## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 10a

13.13

8.28 8.28 7.89 7.89 7.88 7.87 7.53 7.53 7.52 7.52 7.51 7.51 7.50 7.50 7.49 7.48 7.47 7.47 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.43 7.42 7.40 7.40 7.40 7.38

3.70

2.51 2.50 2.50 2.50 2.49

1.02

1.00 2.05 8.57

3.00

4.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 10a

159.89

139.92 138.67 133.03 132.34 129.96 129.00 128.54 128.42 128.10 127.66 124.93 116.02 107.03 105.08

68.15

50.85 40.13 39.92 39.71 39.50 39.29 39.08 38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S28

NOESY spectra (DMSO-d_6, 400 MHz) of compound **10a**

¹H NMR spectra (DMSO-*d*₆, 400 MHz) of compound **10b**

13.25

8.40
8.37
8.00
7.95
7.93
7.93
7.92
7.92
7.91
7.58
7.57
7.56
7.55
7.55
7.54
7.54
7.54
7.53
7.52
7.52
7.48
7.48
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.42

3.71

2.51
2.50
2.50

1.04

2.04
1.98
2.06
4.00
3.11

3.00

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

¹³C NMR spectra (DMSO-*d*₆, 100 MHz) of compound **10b**

159.88
140.09
138.74
133.04
132.91
132.55
132.34
129.97
128.59
128.11
127.87
127.67
126.89
126.52
126.00
123.27
123.04
116.01
107.63
105.15

68.16

50.87
40.13
39.92
39.71
39.50
39.29
39.19
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

S30

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 10c

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 10c
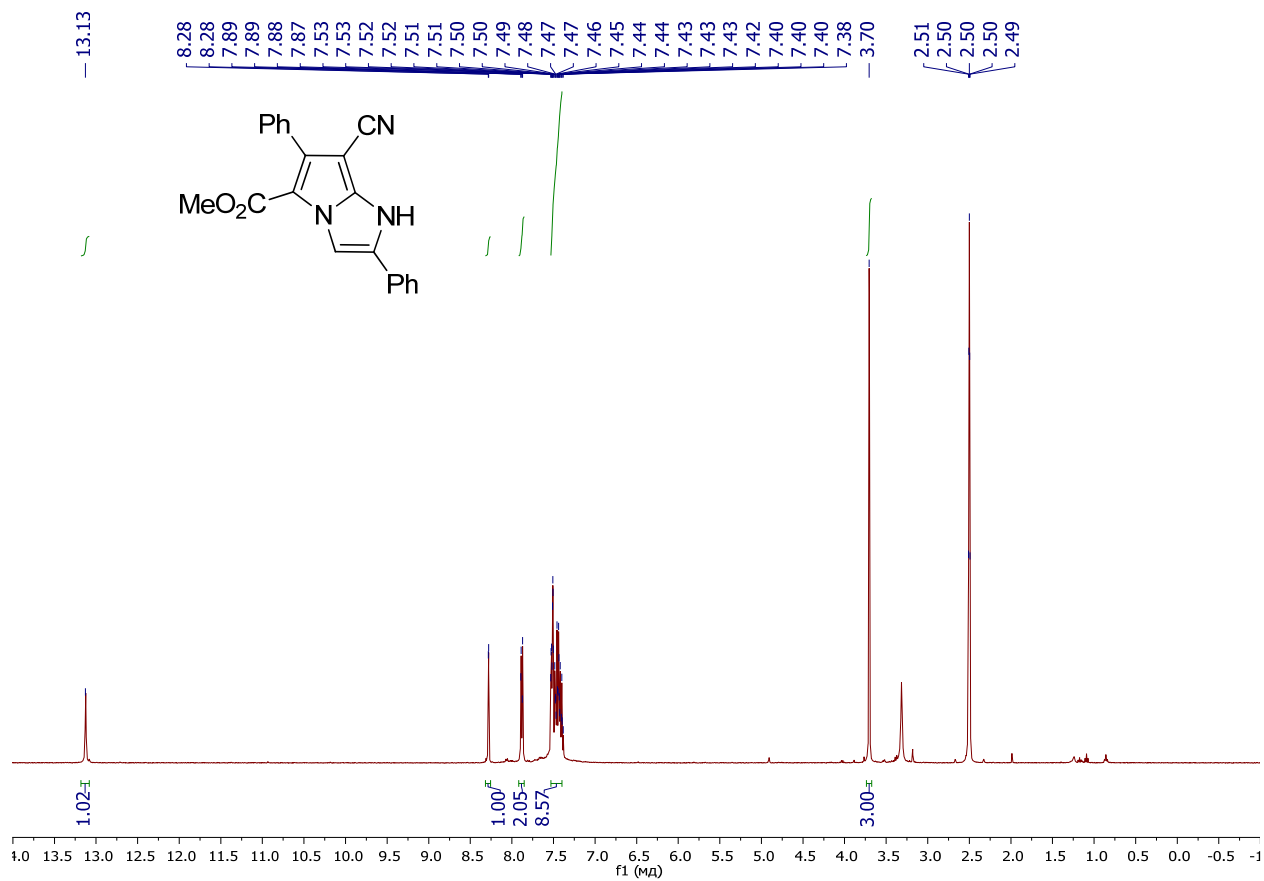
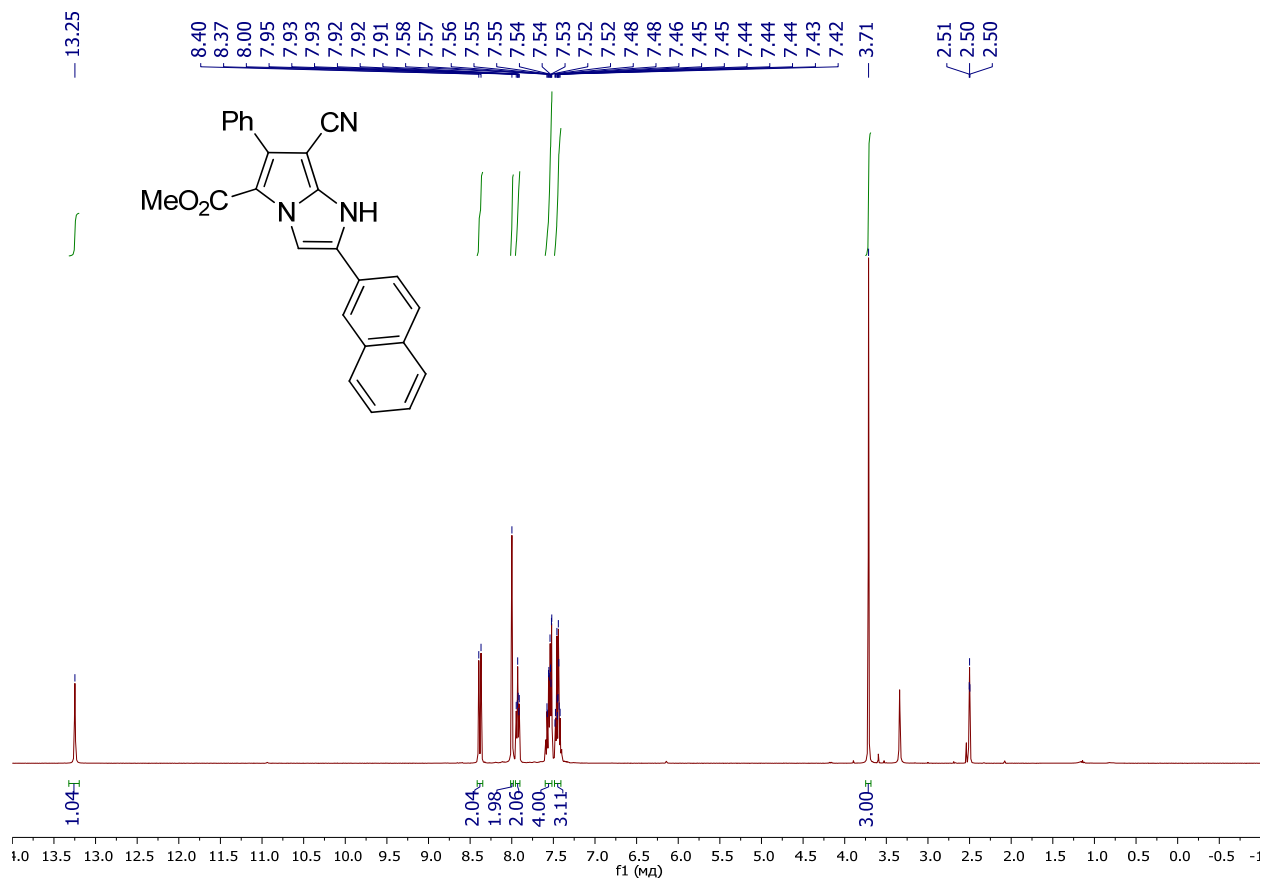## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **10d**

13.11

8.25
7.93
7.92
7.91
7.90
7.53
7.52
7.51
7.51
7.50
7.50
7.50
7.47
7.47
7.45
7.43
7.43
7.42
7.42
7.41
7.36
7.34
7.32

3.69

2.50
2.50
2.50

0.93

0.95
2.04
2.02
3.27
2.29

3.00

1.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **10d**

163.22
160.78
159.87
139.90
138.62
132.33
132.17
129.95
128.11
127.67
127.22
127.14
125.19
125.16
116.01
116.10
115.89
107.03
105.10

68.12

50.86
40.13
39.92
39.71
39.50
39.29
39.08
38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 10e

13.13

8.13, 7.84, 7.82, 7.73, 7.72, 7.71, 7.70, 7.57, 7.55, 7.54, 7.53, 7.52, 7.52, 7.48, 7.48, 7.46, 7.44, 7.43, 7.42, 7.42, 7.41, 7.40, 7.40, 7.39

3.67

2.51, 2.50, 2.50, 2.50, 2.49

0.92

0.90, 0.98, 1.01, 3.11, 4.36

3.00

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 10e

159.99, 139.30, 138.81, 133.58, 132.31, 131.56, 130.94, 130.82, 129.94, 129.31, 128.14, 128.03, 127.67, 121.78, 115.85, 109.69, 104.91

68.04

50.88, 40.13, 39.92, 39.71, 39.50, 39.29, 39.08, 38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound 10f

13.15

8.17
7.80
7.79
7.78
7.77
7.66
7.66
7.64
7.64
7.54
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.47
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.42

3.67

2.50
2.50
2.50
2.49

1.02

0.90
1.01
1.05
7.47

3.00

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound 10f

160.01
139.39
138.90
132.29
131.13
130.53
130.50
130.33
129.94
129.35
128.16
127.67
127.62
127.12
115.85
109.97
104.93

68.07

50.88
40.13
39.92
39.71
39.50
39.29
39.08
38.88

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
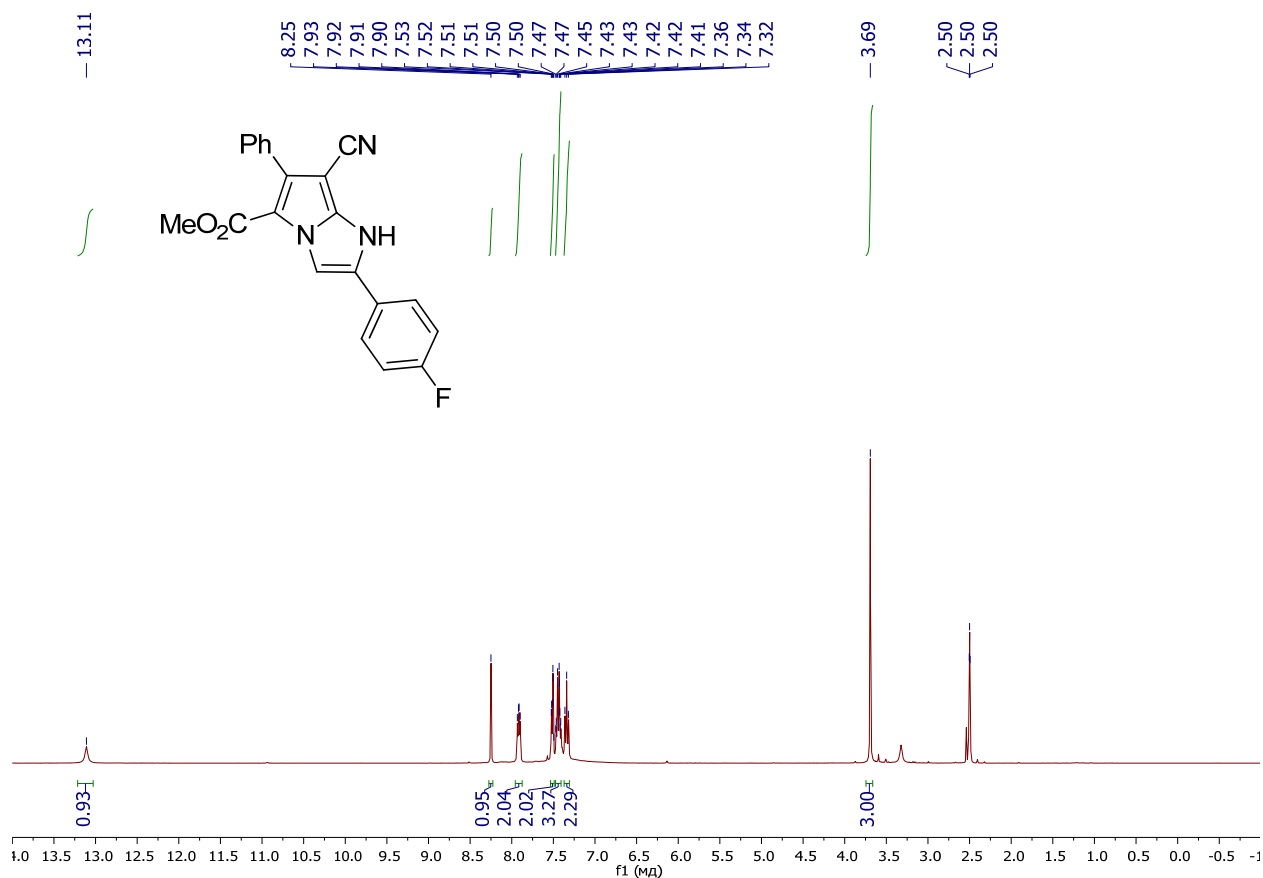f1 (мд)

S34

^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **10g**

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **10g**

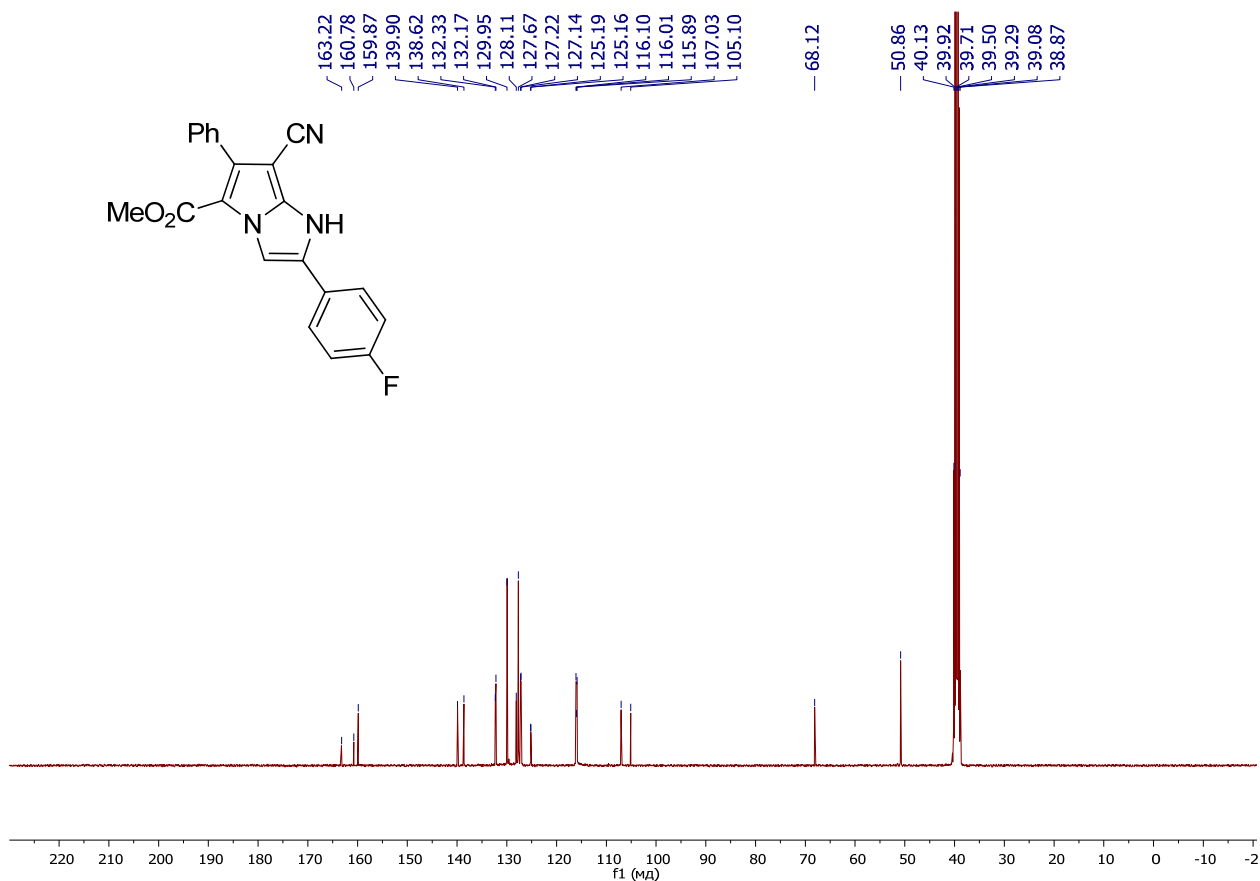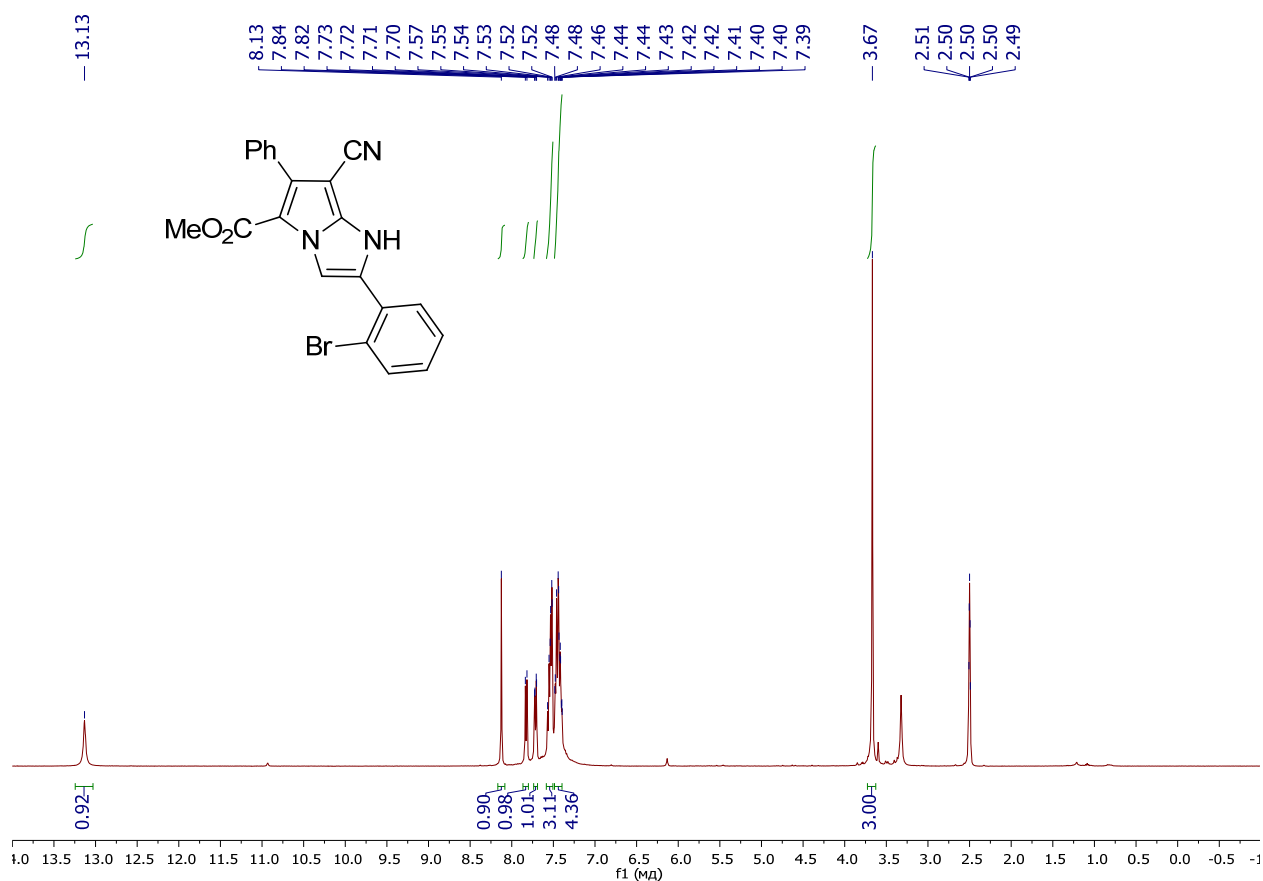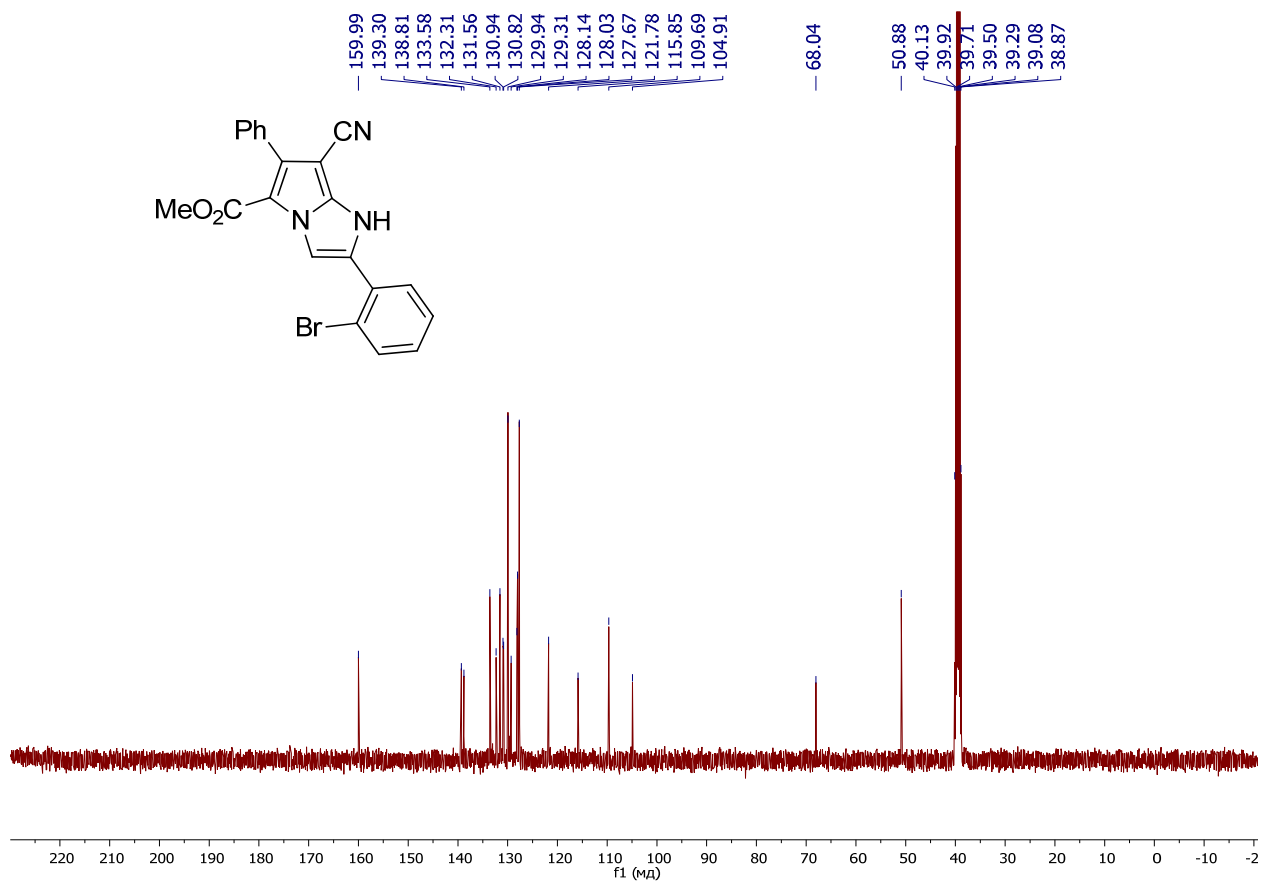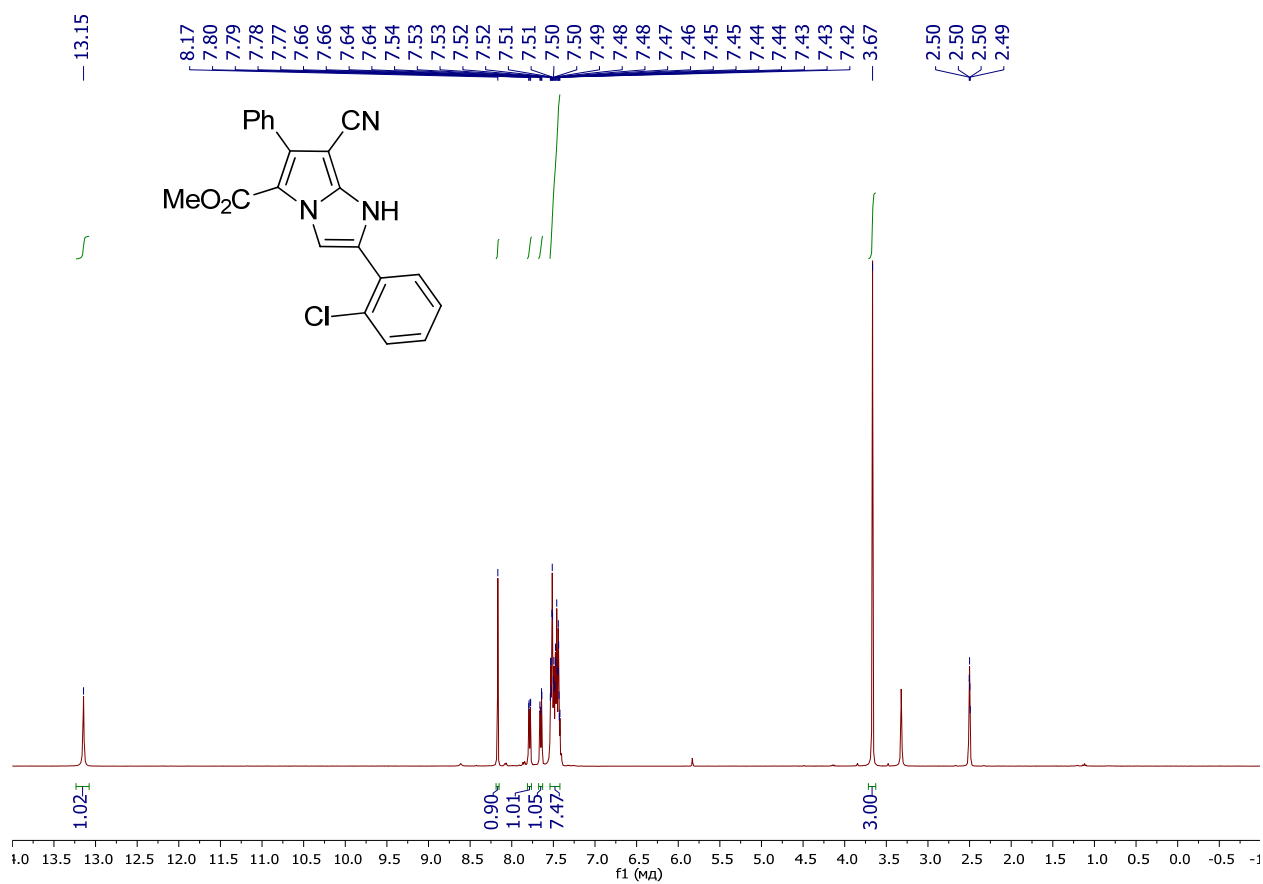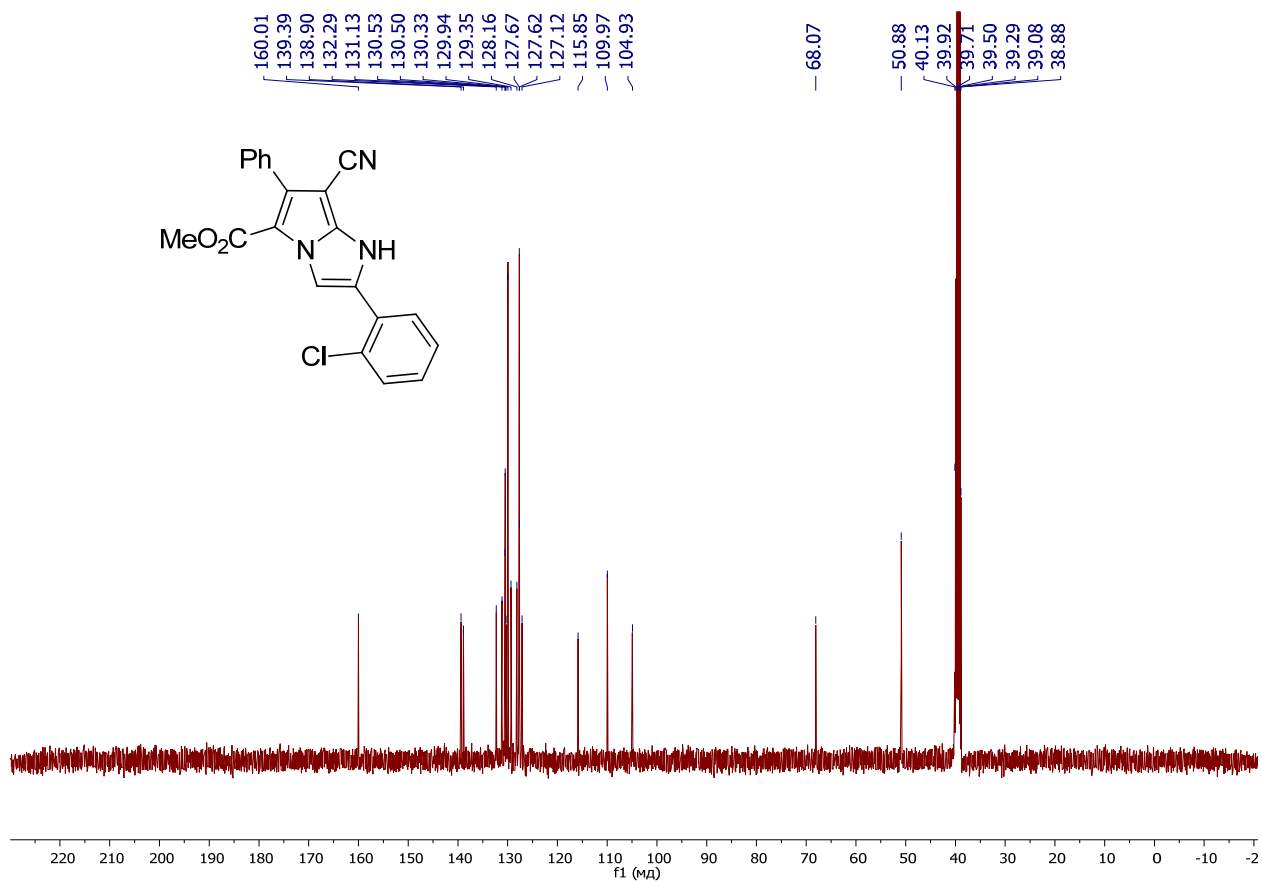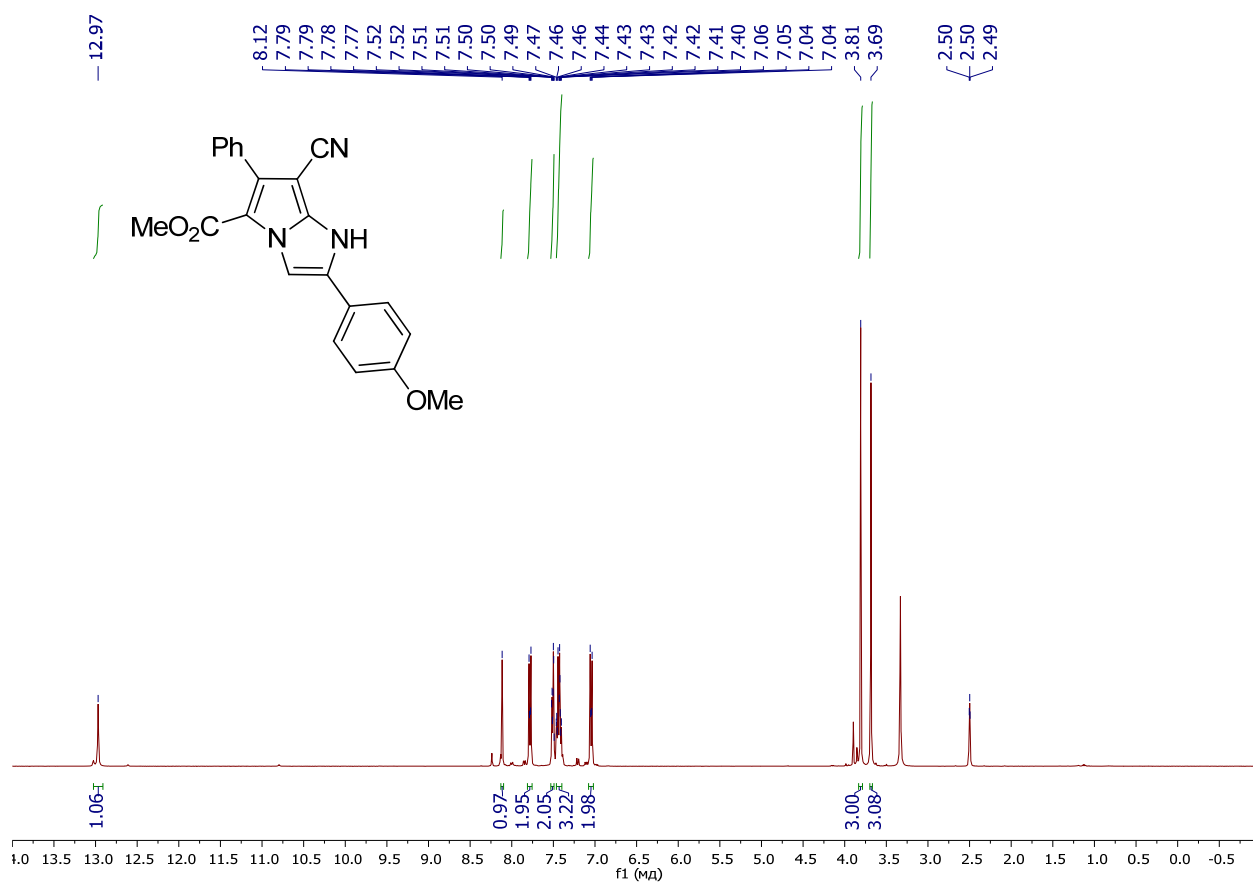## ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **10h**

13.06

8.22
7.77
7.75
7.53
7.52
7.51
7.50
7.47
7.45
7.43
7.41
7.32
7.30

3.70

2.51
2.51
2.50
2.50
2.49
2.35

1.02
1.03
2.02
5.43
2.03
3.00
3.02

4.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **10h**

159.89
139.77
138.54
137.99
133.14
132.36
129.95
129.53
128.07
127.65
125.74
124.85
116.04
106.50
105.04

68.11

50.83
40.13
39.92
39.71
39.50
39.29
39.08
38.87
20.79

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

^{1}H NMR spectra (CDCl$_3$, 400 MHz) of compound **12**

7.96, 7.96, 7.94, 7.94, 7.91, 7.67, 7.67, 7.66, 7.65, 7.65, 7.64, 7.63, 7.63, 7.62, 7.59, 7.59, 7.58, 7.57, 7.57, 7.56, 7.53, 7.53, 7.51, 7.49, 7.49, 7.48, 7.47, 7.46, 7.46, 7.45, 7.44, 7.43, 7.43, 7.42, 7.42, 7.41, 7.28, 5.56, 3.79

2.01, 0.86, 1.08, 1.97, 10.14, 1.99, 3.00

^{13}C NMR spectra (CDCl$_3$, 100 MHz) of compound **12**

191.68, 161.08, 140.86, 139.47, 135.32, 134.45, 133.72, 132.32, 130.16, 129.76, 129.40, 129.23, 129.08, 128.31, 128.15, 127.81, 127.31, 115.84, 109.43, 106.47, 77.37, 77.05, 76.73, 69.25, 51.08, 50.44

¹H NMR spectra (DMSO-*d*₆, 400 MHz) of compound **14a**

¹³C NMR spectra (DMSO-*d*₆, 100 MHz) of compound **14a**

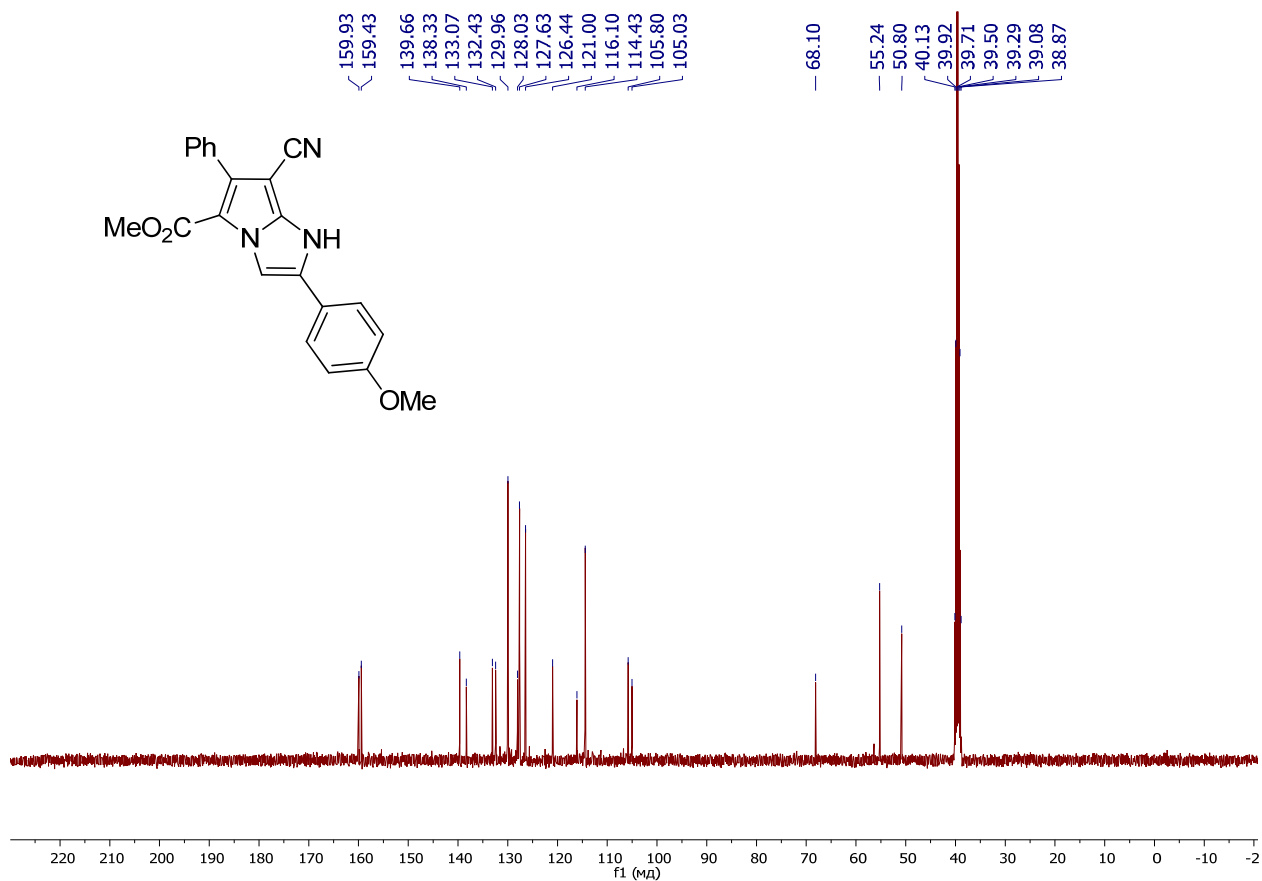# ¹H NMR spectra (DMSO-*d*₆, 400 MHz) of compound **14b**
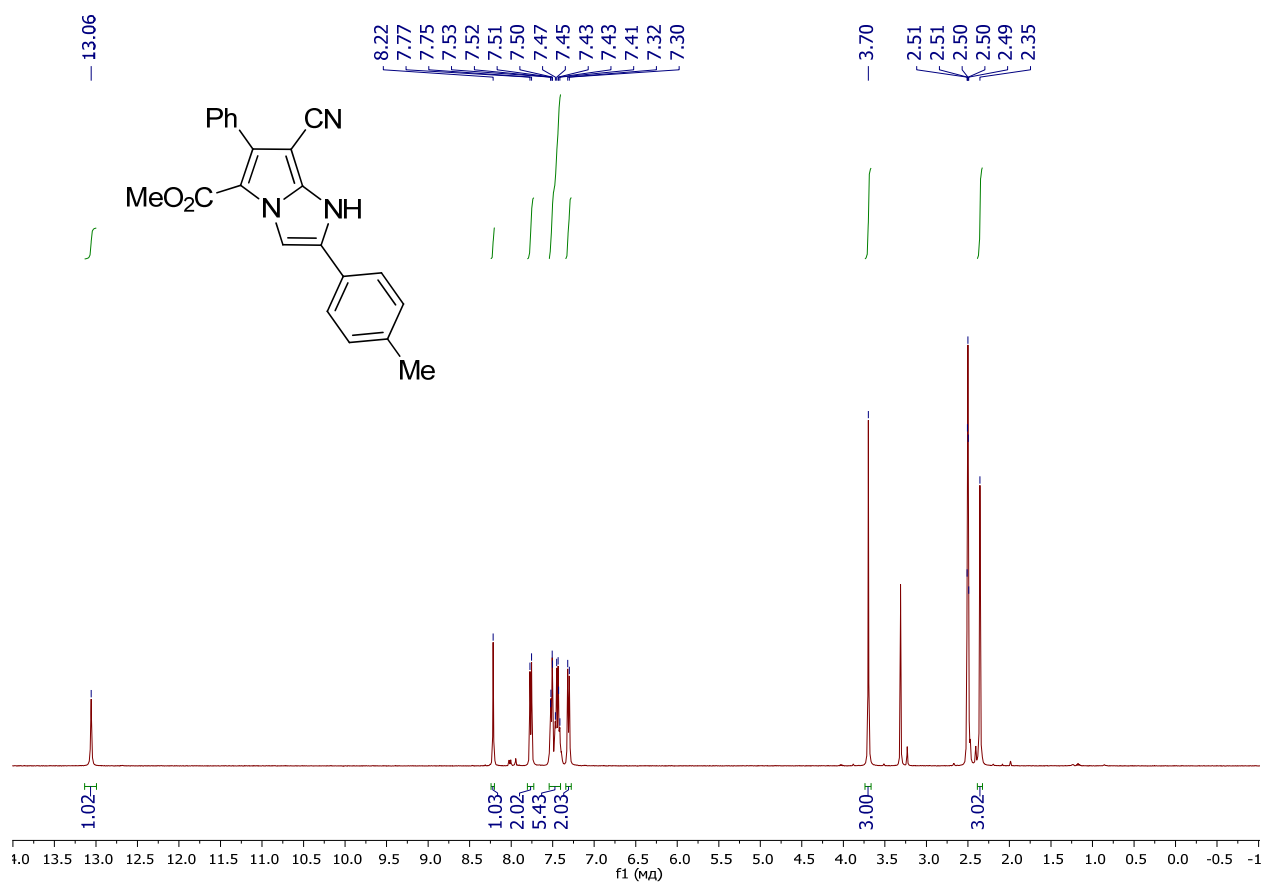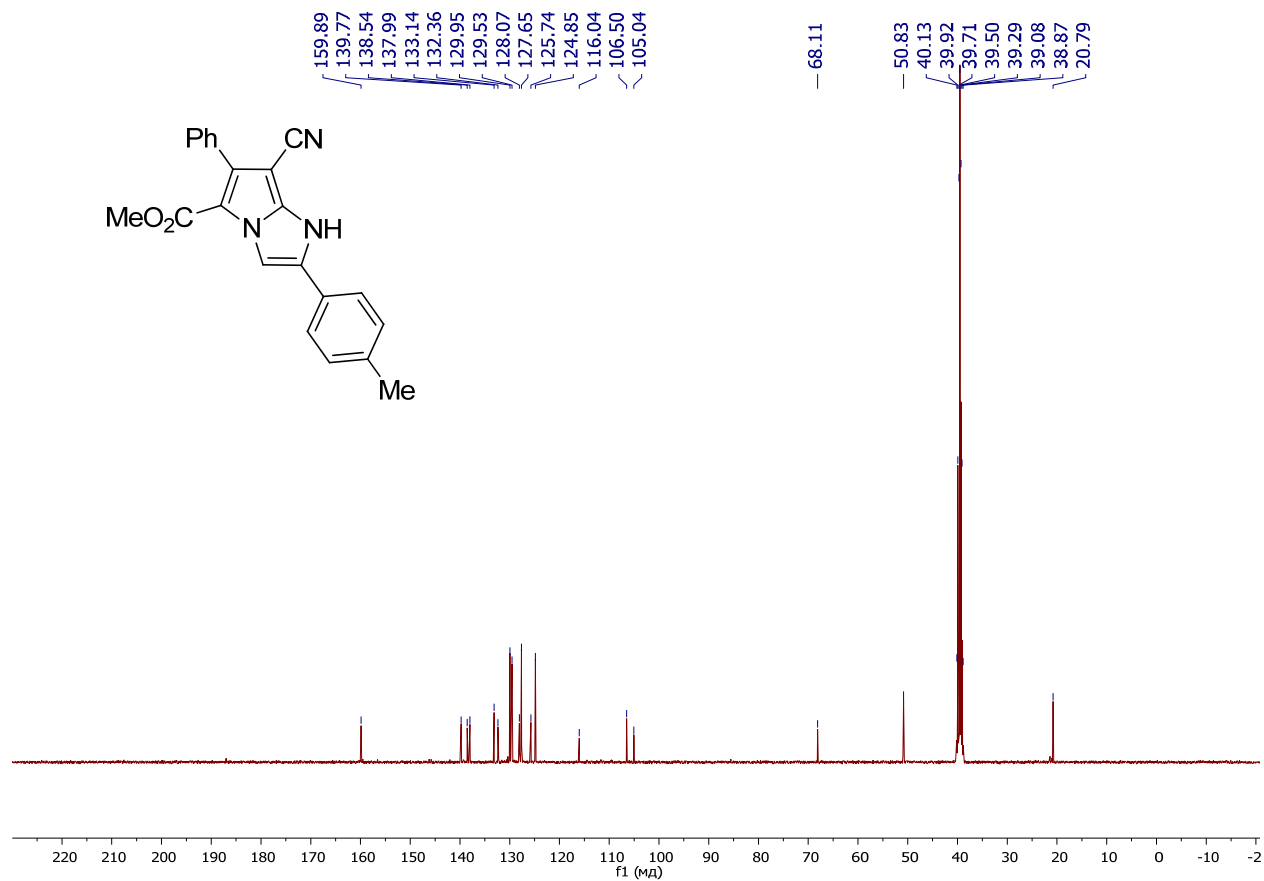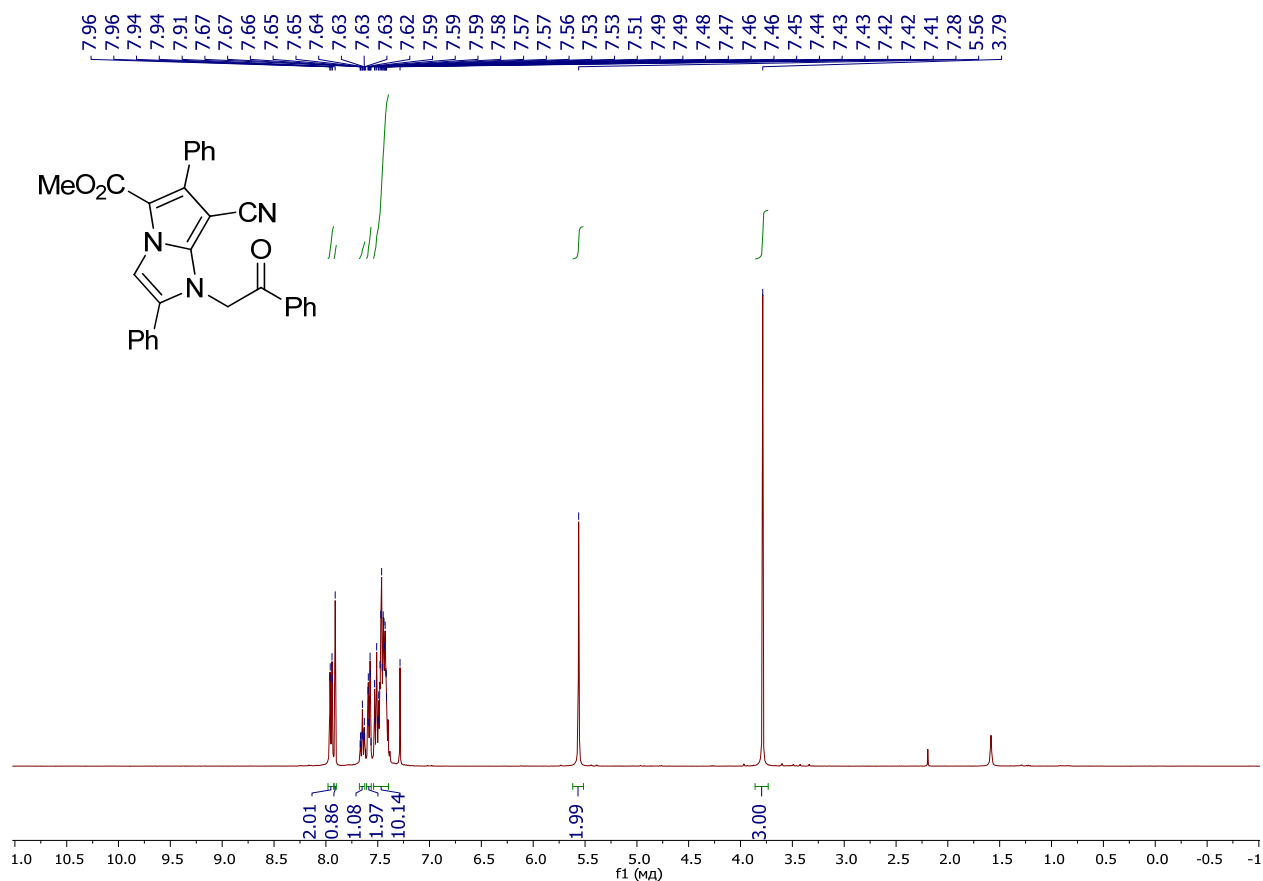
^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **14b**

12.52

8.19 7.66 7.66 7.64 7.64 7.38 7.38 7.37 7.36

3.66 3.33

2.51 2.50 2.50

1.00 — 1.03 — 2.11 — 2.12 — 3.00 —

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (мд)

^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **14b**

160.76 158.48 154.72 150.32

132.73 132.14 131.06 121.31 121.03 120.06

101.84

51.49 40.13 39.92 39.82 39.71 39.50 39.29 39.17 39.08 38.87

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (мд)

H NMR spectra (DMSO-d_6, 400 MHz) of compound **14c**

C NMR spectra (DMSO-d_6, 100 MHz) of compound **14c**
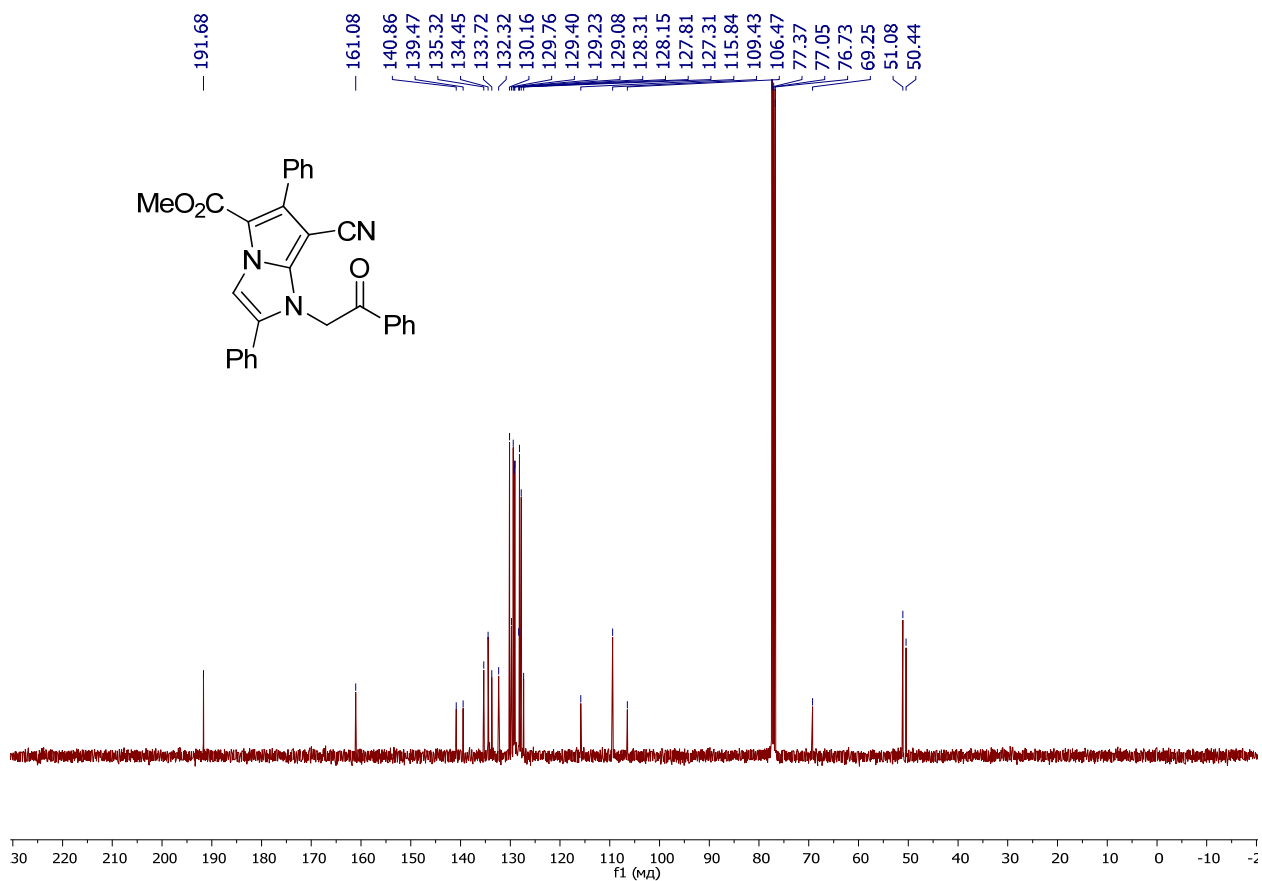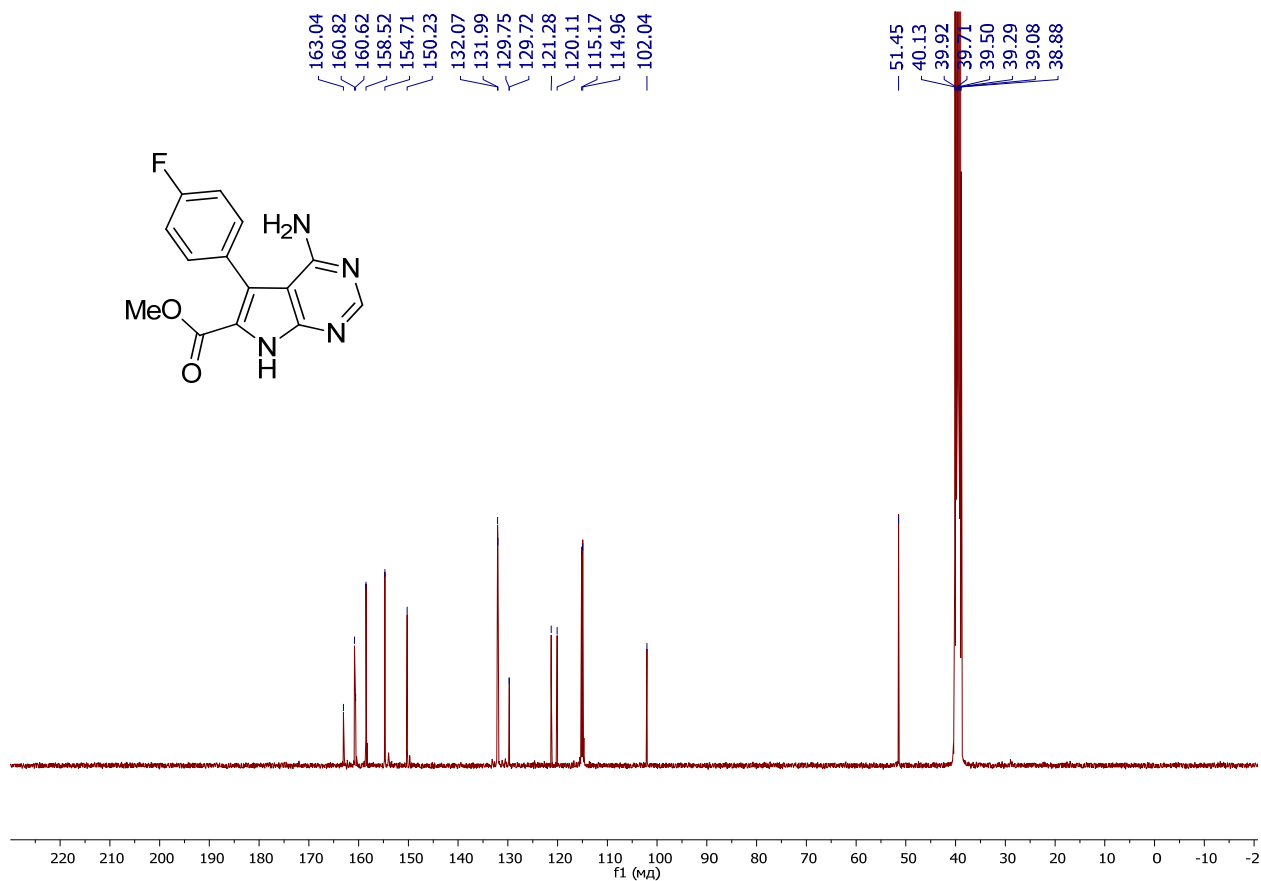
^{1}H NMR spectra (DMSO-d_6, 400 MHz) of compound **14d**

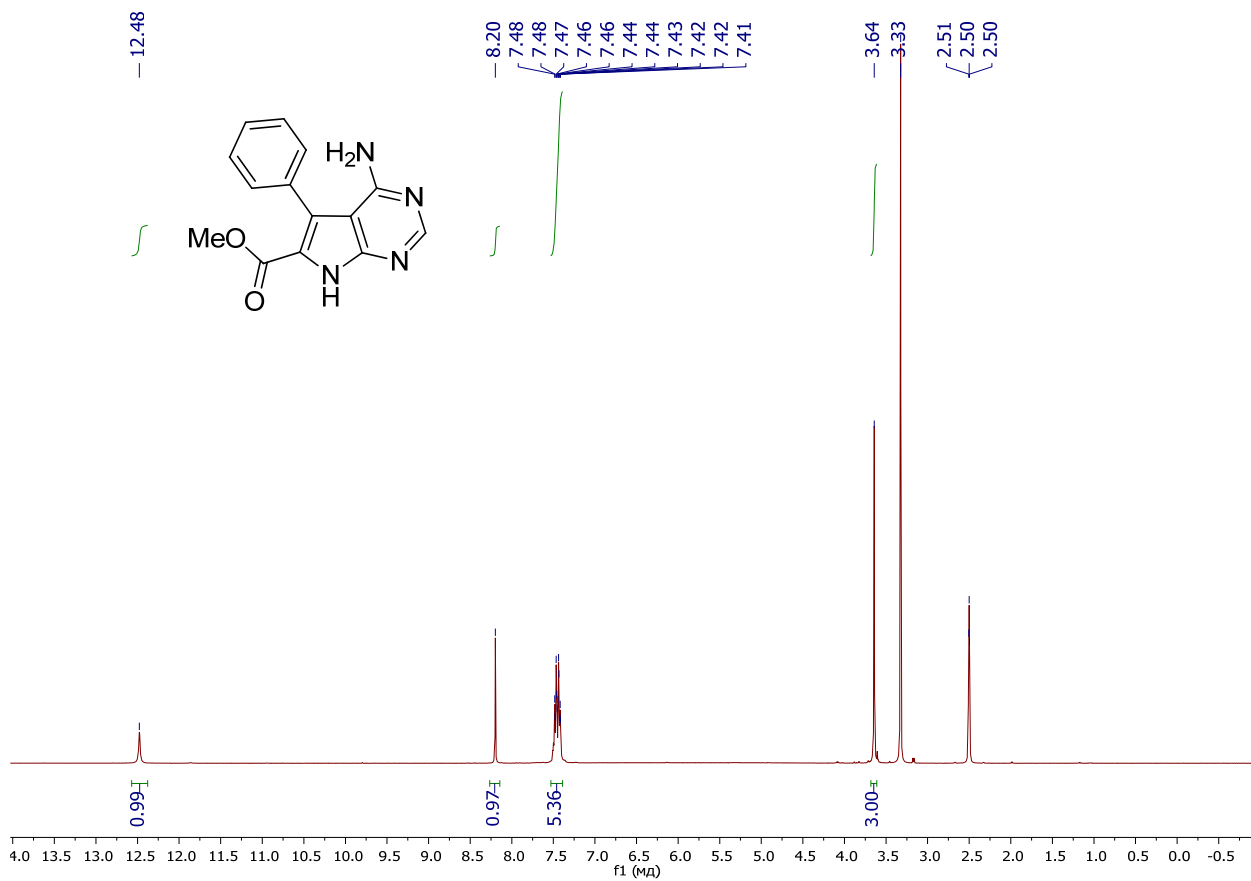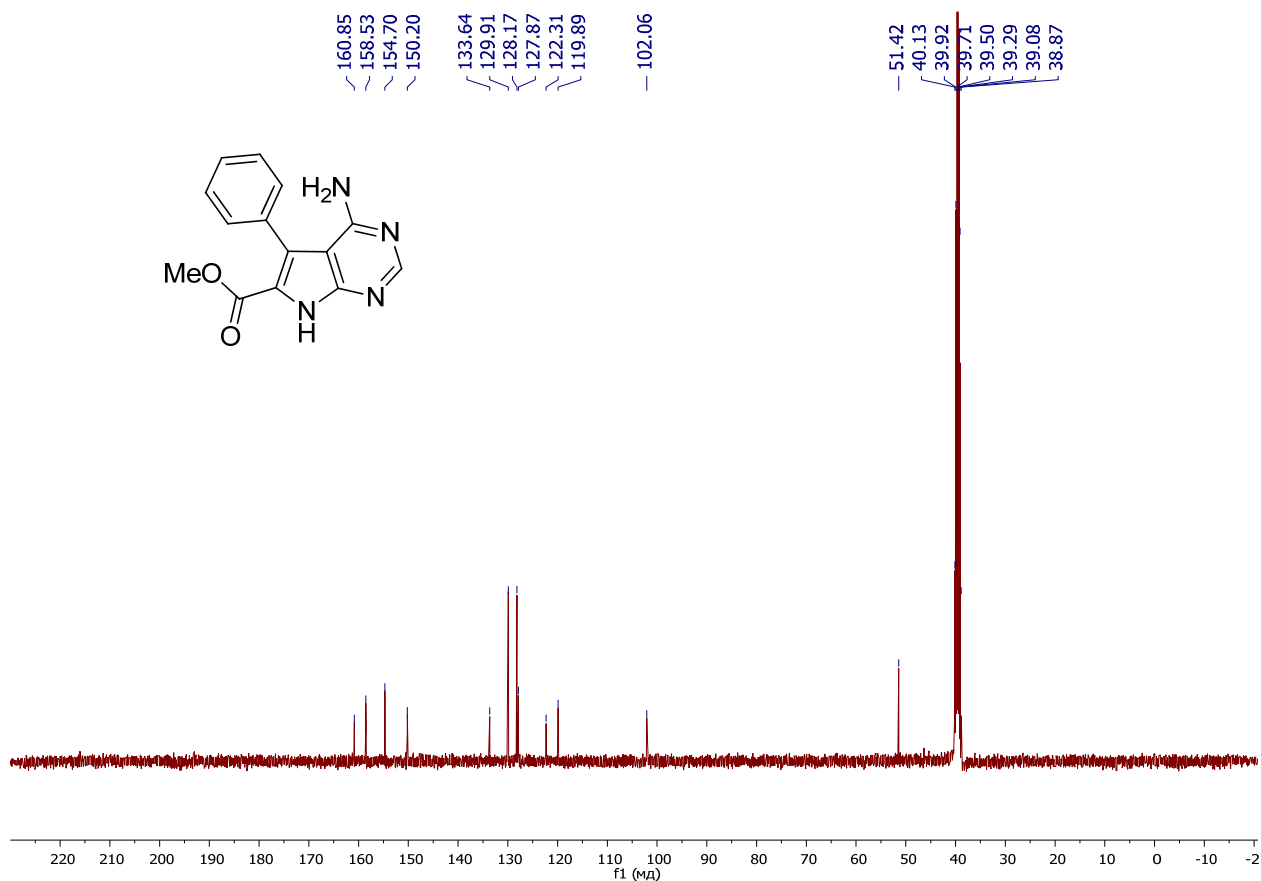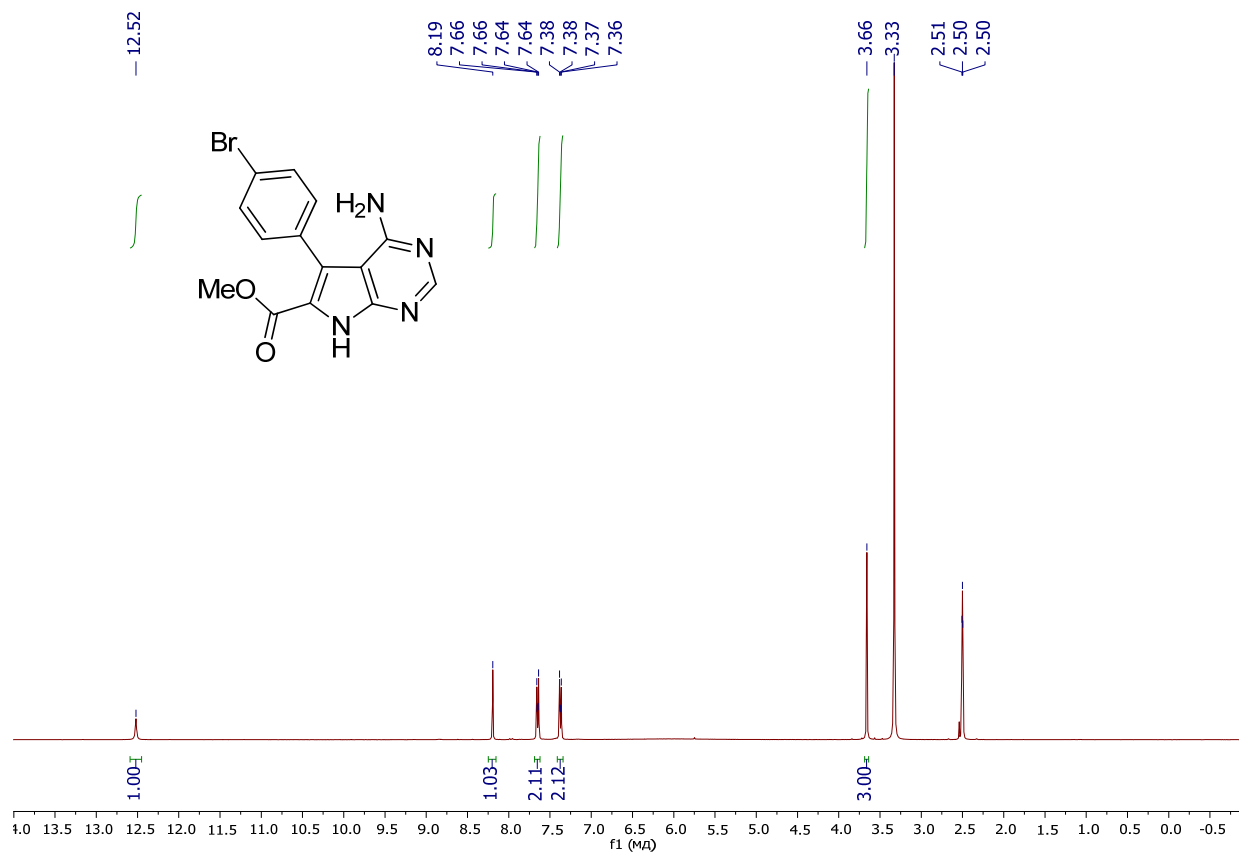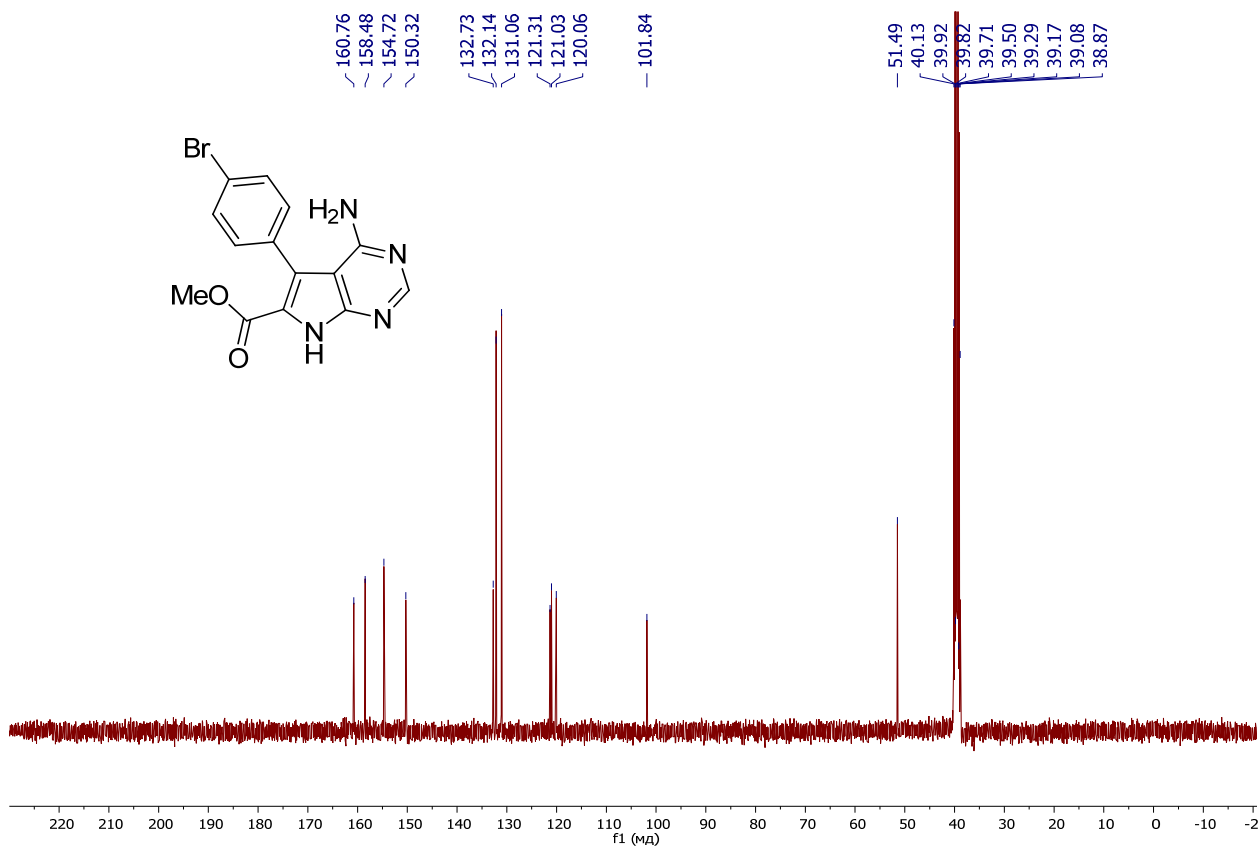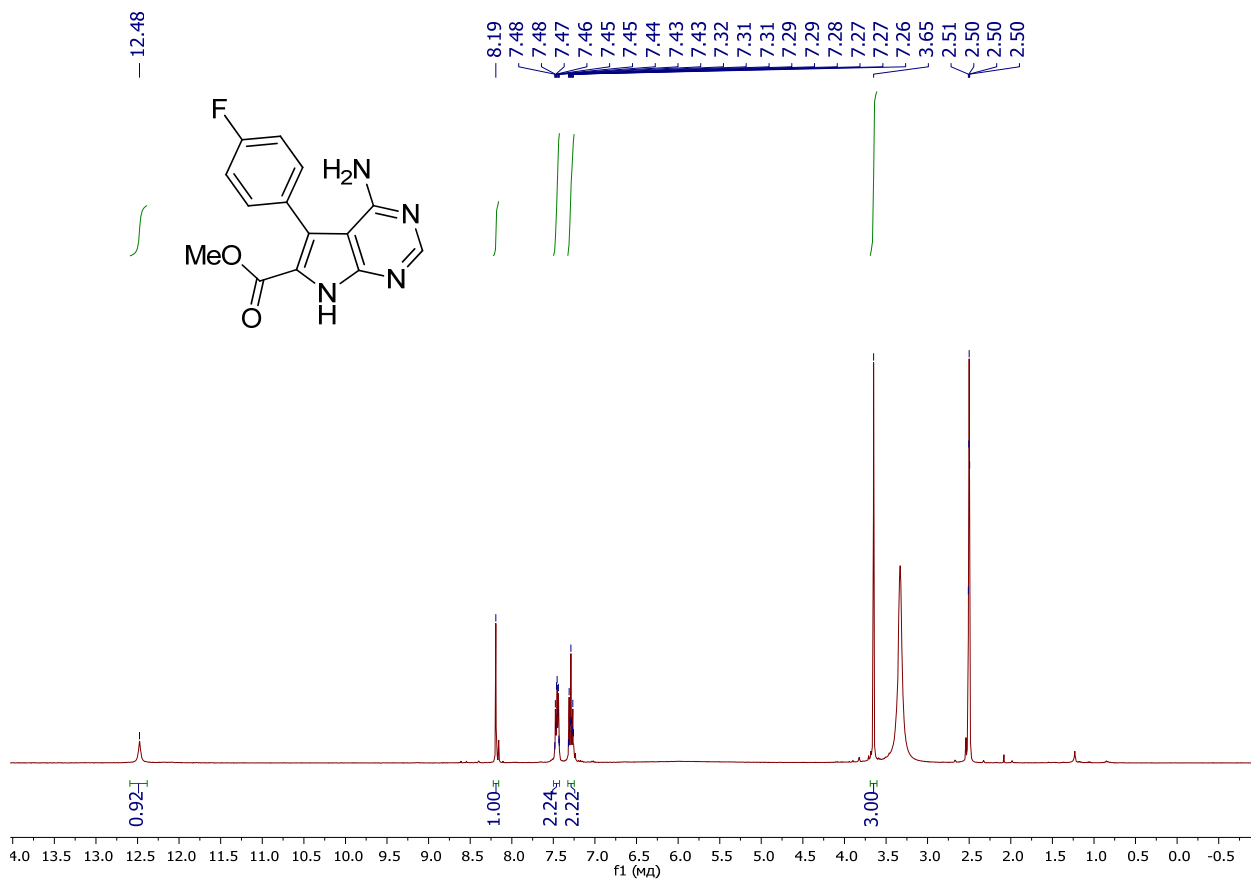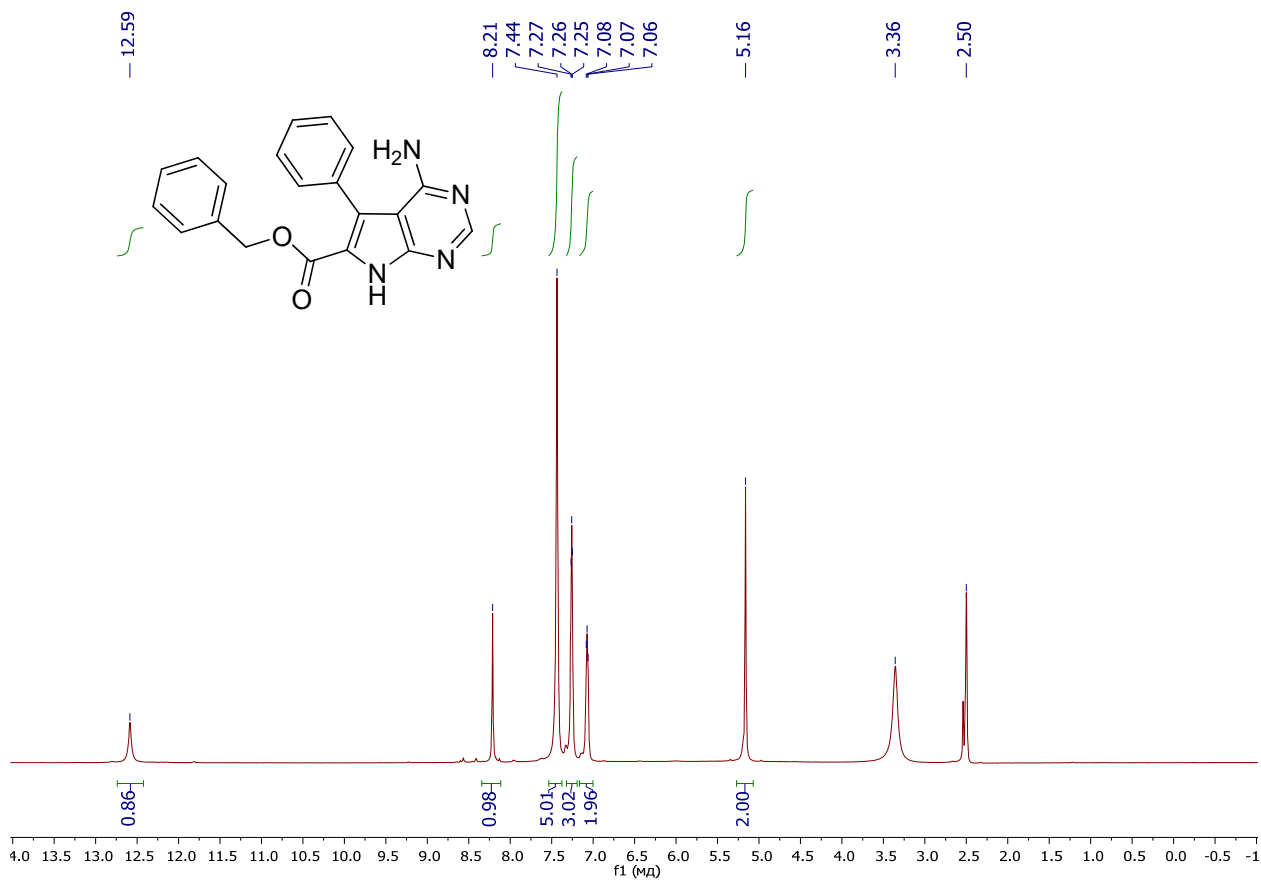# ^{13}C NMR spectra (DMSO-d_6, 100 MHz) of compound **14d**
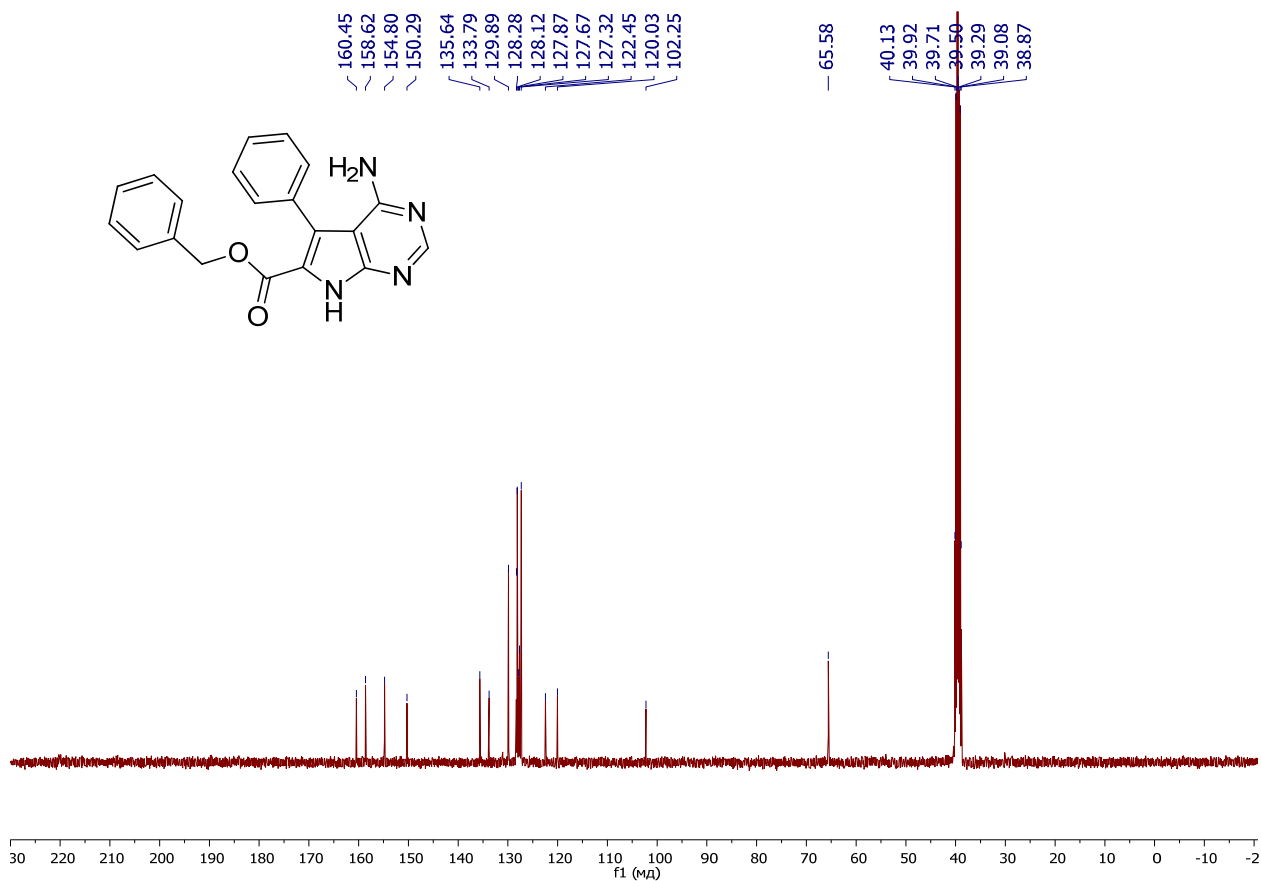
3. X-ray crystal structure of compound 2b

Crystal structure of **2b** was determined by single crystal X-ray diffraction analysis. Suitable crystals were selected and fixed on micro-amounts and the diffraction data were collected on a SuperNova diffractometer. The crystals **2b** were measured at a temperature of 100(1) R, using monochromated CuKα radiation. The unit cell parameters and refinement characteristics of the crystal structure of **2b** is given below. Using Olex2[5], the structure was solved with the ShelXT[6] structure solution program using Intrinsic Phasing and refined with the ShelXL[7] refinement package using Least Squares minimization.

Methyl 5-amino-4-cyano-3-phenyl-1*H*-pyrrole-2-carboxylate 2b (CCDC 2053975)
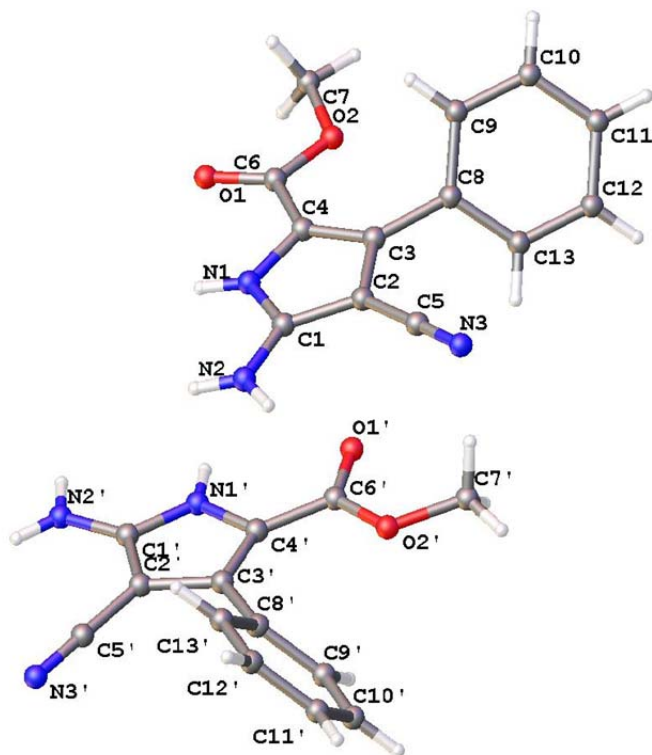
Molecular structure of compound **2b**, displacement parameters are drawn at 50% probability level.

Table S2. Crystal data and structure refinement for 7060-11161_lia501.

Identification code	7060-11161_lia501
Empirical formula	$C_{13}H_{11}N_3O_2$
Formula weight	241.25
Temperature/K	99.99(13)
Crystal system	triclinic
Space group	P-1
a/Å	7.2529(3)
b/Å	12.9297(5)
c/Å	13.0243(5)
α/°	85.469(3)
β/°	82.621(3)
γ/°	73.765(3)
Volume/Å^3	1161.78(8)
Z	4
ρ_{calc}g/cm^3	1.379
μ/mm^{-1}	0.793
F(000)	504.0
Crystal size/mm^3	0.14 × 0.09 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.85 to 124.98
Index ranges	-8 ≤ h ≤ 8, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
Reflections collected	16032
Independent reflections	3695 [R_{int} = 0.0359, R_{sigma} = 0.0241]
Data/restraints/parameters	3695/0/327
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0341, wR_2 = 0.0881
Final R indexes [all data]	R_1 = 0.0385, wR_2 = 0.0920
Largest diff. peak/hole / e Å^{-3}	0.21/-0.24

Table S3. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 7060-11161_lia501. U$_{eq}$ is defined as 1/3 of of the trace of the orthogonalised U$_{IJ}$ tensor.

Atom	x	y	z	U(eq)
O1	-578.4(15)	5477.4(8)	6445.1(8)	19.5(2)
O2	366.7(15)	4768.5(8)	7992.2(7)	19.0(2)
O2'	8197.3(16)	2047.6(8)	4738.8(8)	22.4(3)
O1'	6577.1(16)	3608.1(8)	5464.4(8)	22.6(3)
N1	1622.4(17)	3602.8(9)	5495.6(9)	15.6(3)
N1'	5558.1(18)	4527.5(10)	3546.1(9)	17.0(3)
N2	3068.6(18)	2304.5(10)	4252.9(9)	19.1(3)
N3	5018(2)	14.2(10)	6265.1(10)	22.9(3)
N2'	4085.2(19)	5732.7(10)	2246.4(10)	20.8(3)
N3'	6279(2)	3721.5(11)	30.6(10)	25.5(3)
C3	2393(2)	2722.2(11)	7005.2(11)	14.8(3)
C1	2689(2)	2608.3(11)	5238.0(11)	14.2(3)
C2	3205(2)	2026.2(11)	6162.2(11)	14.9(3)
C1'	5189(2)	4765.8(12)	2558.4(11)	16.6(3)
C8'	8114(2)	1911.8(11)	2407.9(10)	15.8(3)
C5	4201(2)	916.6(12)	6228.3(11)	16.1(3)
C6'	7130(2)	3065.5(12)	4698.9(11)	16.6(3)
C8	2628(2)	2381.9(11)	8103.2(11)	15.3(3)
C2'	6089(2)	3835.4(12)	2003.0(11)	16.1(3)
C13	4466(2)	1872.1(11)	8384.5(11)	17.0(3)
C9'	9988(2)	1430.3(12)	2649.3(11)	17.4(3)
C9	1045(2)	2510.1(11)	8860.2(11)	17.2(3)
C10'	10977(2)	411.4(12)	2316.0(11)	19.5(3)
C13'	7258(2)	1350.7(12)	1826.3(11)	18.4(3)
C6	309(2)	4724.8(11)	6980.1(11)	15.1(3)
C4'	6687(2)	3468.8(11)	3665.2(11)	16.5(3)
C4	1411(2)	3696.6(12)	6567.9(11)	16.0(3)
C5'	6187(2)	3769.8(11)	914.8(12)	17.8(3)
C3'	7041(2)	3014.1(11)	2710.0(11)	15.5(3)
C12	4730(2)	1498.2(12)	9397.0(12)	20.5(3)
C10	1311(2)	2121.5(12)	9869.9(11)	19.5(3)
C12'	8242(2)	327.9(12)	1502.7(12)	21.1(3)
C11	3149(2)	1616.7(12)	10140.5(11)	20.6(3)
C11'	10106(2)	-140.3(12)	1744.3(12)	21.6(3)
C7'	8711(2)	1595.7(13)	5746.0(11)	23.2(3)
C7	-802(2)	5742.1(12)	8473.4(12)	21.8(3)

Table S4. Anisotropic Displacement Parameters (Å$^2 \times 10^3$) for 7060-11161_lia501. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	22.7(6)	13.5(5)	18.1(5)	0.1(4)	-3.6(4)	2.2(4)
O2	24.1(6)	12.9(5)	16.3(5)	-3.1(4)	-3.9(4)	2.4(4)
O2'	29.5(6)	17.9(5)	14.3(5)	1.1(4)	-4.0(4)	2.6(5)
O1'	28.1(6)	20.9(5)	15.2(5)	-3.4(4)	-3.8(4)	0.3(5)
N1	17.8(6)	11.7(6)	14.5(6)	1.2(5)	-4.0(5)	1.1(5)
N1'	20.8(7)	15.3(6)	12.8(6)	-3.0(5)	-2.3(5)	-0.9(5)
N2	23.9(7)	14.5(6)	14.8(6)	-1.3(5)	-3.1(5)	2.2(5)
N3	29.2(7)	16.7(7)	17.8(7)	-2.1(5)	-3.8(5)	2.5(6)
N2'	26.8(7)	16.2(6)	14.1(6)	-2.5(5)	-3.9(5)	4.2(5)
N3'	33.7(8)	21.5(7)	15.7(7)	-0.7(5)	-4.8(6)	2.5(6)
C3	13.0(7)	13.6(7)	16.6(7)	-1.2(6)	-2.2(6)	-1.3(6)
C1	12.5(7)	12.7(7)	16.3(7)	-1.3(6)	-1.4(6)	-1.3(6)
C2	13.3(7)	13.0(7)	16.9(7)	-1.4(6)	-2.2(6)	-0.5(6)
C1'	16.5(7)	17.9(7)	15.2(7)	0.1(6)	-2.0(6)	-4.1(6)
C8'	18.9(7)	16.1(7)	10.4(7)	1.4(5)	0.2(6)	-2.8(6)
C5	16.8(7)	18.3(8)	11.9(7)	-1.7(6)	-3.3(6)	-1.7(6)
C6'	14.6(7)	17.3(7)	17.1(7)	-1.3(6)	-1.6(6)	-3.0(6)
C8	19.3(8)	9.0(7)	16.7(7)	-2.0(5)	-2.8(6)	-1.6(6)
C2'	15.6(7)	17.3(7)	14.2(7)	-0.9(6)	-2.4(6)	-2.3(6)
C13	17.8(7)	15.2(7)	16.4(7)	-2.2(6)	-1.1(6)	-1.8(6)
C9'	20.3(8)	18.6(7)	13.0(7)	0.4(6)	-2.9(6)	-4.6(6)
C9	17.3(8)	12.7(7)	20.5(7)	-3.1(6)	-3.0(6)	-1.0(6)
C10'	17.1(8)	19.4(8)	17.9(7)	3.1(6)	-2.5(6)	0.8(6)
C13'	17.6(8)	19.3(7)	16.9(7)	1.5(6)	-3.4(6)	-2.6(6)
C6	14.4(7)	14.2(7)	15.5(7)	0.3(6)	-1.8(6)	-2.2(6)
C4'	16.8(7)	14.6(7)	16.8(7)	-0.1(6)	-2.8(6)	-1.9(6)
C4	17.0(7)	14.8(7)	14.5(7)	-1.7(6)	-2.0(6)	-1.0(6)
C5'	16.0(7)	12.5(7)	21.5(9)	-0.4(6)	-2.3(6)	1.9(6)
C3'	13.6(7)	16.6(7)	15.8(7)	-0.1(6)	-1.7(6)	-3.6(6)
C12	19.7(8)	19.9(8)	21.1(8)	-0.1(6)	-6.5(6)	-2.2(6)
C10	24.1(8)	16.6(7)	16.8(7)	-4.6(6)	2.9(6)	-5.2(6)
C12'	26.2(8)	17.7(8)	19.8(8)	-2.2(6)	-3.8(6)	-5.8(7)
C11	29.1(9)	18.9(8)	14.2(7)	0.6(6)	-4.8(6)	-6.4(7)
C11'	26.4(9)	13.5(7)	20.9(8)	-0.7(6)	-0.1(6)	0.0(7)
C7'	24.1(8)	25.3(8)	16.3(7)	6.1(6)	-5.0(6)	-1.4(7)
C7	24.5(8)	17.3(8)	20.3(8)	-7.0(6)	-0.1(6)	0.4(6)

Table S5. Bond Lengths for 7060-11161_lia501.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C6	1.2266(17)	C1'	C2'	1.405(2)
O2	C6	1.3304(17)	C8'	C9'	1.393(2)
O2	C7	1.4448(17)	C8'	C13'	1.395(2)
O2'	C6'	1.3281(18)	C8'	C3'	1.477(2)
O2'	C7'	1.4435(17)	C6'	C4'	1.447(2)
O1'	C6'	1.2238(18)	C8	C13	1.394(2)
N1	C1	1.3451(18)	C8	C9	1.395(2)
N1	C4	1.3965(19)	C2'	C5'	1.418(2)
N1'	C1'	1.3422(19)	C2'	C3'	1.432(2)
N1'	C4'	1.3931(19)	C13	C12	1.386(2)
N2	C1	1.3434(19)	C9'	C10'	1.386(2)
N3	C5	1.1519(19)	C9	C10	1.388(2)
N2'	C1'	1.3462(19)	C10'	C11'	1.386(2)
N3'	C5'	1.151(2)	C13'	C12'	1.385(2)
C3	C2	1.434(2)	C6	C4	1.450(2)
C3	C8	1.480(2)	C4'	C3'	1.381(2)
C3	C4	1.381(2)	C12	C11	1.384(2)
C1	C2	1.404(2)	C10	C11	1.388(2)
C2	C5	1.416(2)	C12'	C11'	1.383(2)

Table S6. Bond Angles for 7060-11161_lia501.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	O2	C7	116.48(11)	C1'	C2'	C5'	125.19(13)
C6'	O2'	C7'	116.53(11)	C1'	C2'	C3'	108.03(13)
C1	N1	C4	110.62(12)	C5'	C2'	C3'	126.50(13)
C1'	N1'	C4'	110.85(12)	C12	C13	C8	120.97(14)
C2	C3	C8	123.42(12)	C10'	C9'	C8'	120.36(14)
C4	C3	C2	106.21(12)	C10	C9	C8	120.10(14)
C4	C3	C8	130.37(13)	C11'	C10'	C9'	120.25(14)
N1	C1	C2	107.16(12)	C12'	C13'	C8'	120.74(14)
N2	C1	N1	122.32(13)	O1	C6	O2	123.63(13)
N2	C1	C2	130.50(13)	O1	C6	C4	123.15(13)
C1	C2	C3	108.06(12)	O2	C6	C4	113.22(12)
C1	C2	C5	124.51(13)	N1'	C4'	C6'	117.77(13)
C5	C2	C3	127.19(13)	C3'	C4'	N1'	107.88(12)
N1'	C1'	N2'	122.44(13)	C3'	C4'	C6'	134.22(13)
N1'	C1'	C2'	107.05(12)	N1	C4	C6	117.89(12)
N2'	C1'	C2'	130.48(14)	C3	C4	N1	107.95(12)
C9'	C8'	C13'	118.81(13)	C3	C4	C6	134.15(13)
C9'	C8'	C3'	122.02(13)	N3'	C5'	C2'	179.36(17)
C13'	C8'	C3'	119.11(13)	C2'	C3'	C8'	123.54(13)
N3	C5	C2	178.90(15)	C4'	C3'	C8'	130.25(13)
O2'	C6'	C4'	113.55(12)	C4'	C3'	C2'	106.20(12)
O1'	C6'	O2'	123.08(13)	C11	C12	C13	119.83(14)
O1'	C6'	C4'	123.38(13)	C9	C10	C11	120.53(14)
C13	C8	C3	119.37(13)	C11'	C12'	C13'	119.89(14)
C13	C8	C9	118.82(13)	C12	C11	C10	119.75(14)
C9	C8	C3	121.74(13)	C12'	C11'	C10'	119.94(14)

Table S7. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 7060-11161_lia501.

Atom	x	y	z	U(eq)
H1	1137.8	4110.54	5060.16	19
H1'	5152.76	4968.8	4038.96	20
H2A	2624.9	2752.26	3760.82	23
H2B	3755.52	1662.28	4114.28	23
H2'A	3587.71	6224.78	2686.39	25
H2'B	3877.83	5858.26	1606.98	25
H13	5530.95	1781.38	7885.65	20
H9'	10578.32	1794.39	3036.41	21
H9	-189.99	2856.52	8687.87	21
H10'	12231.45	96.75	2476.51	23
H13'	6012.12	1666.71	1653.85	22
H12	5967.07	1168.6	9576.33	25
H10	248.61	2199.91	10369.26	23
H12'	7651.09	-43.41	1123.54	25
H11	3318.24	1359.06	10818.81	25
H11'	10772.36	-824.65	1523.29	26
H7'A	9665.82	913.7	5669.04	35
H7'B	7583.44	1494.14	6167.85	35
H7'C	9226.73	2078.67	6070.82	35
H7A	-395.7	6349.15	8154.48	33
H7B	-651.44	5687.32	9199.06	33
H7C	-2134.19	5836.81	8386.52	33

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