New Journal of Chemistry

A long range tautomeric effect on a new Schiff isoniazid analogue, NMR study and X-ray crystallography

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1. **NMR Spectra of the compounds**
2. **X-Ray crystallography of the compounds: Figure 5S, Table 1S, Table 2S, Tables 1-8**
3. **Antibacterial and antifungal activity**
4. **TLC slides from experimental part**

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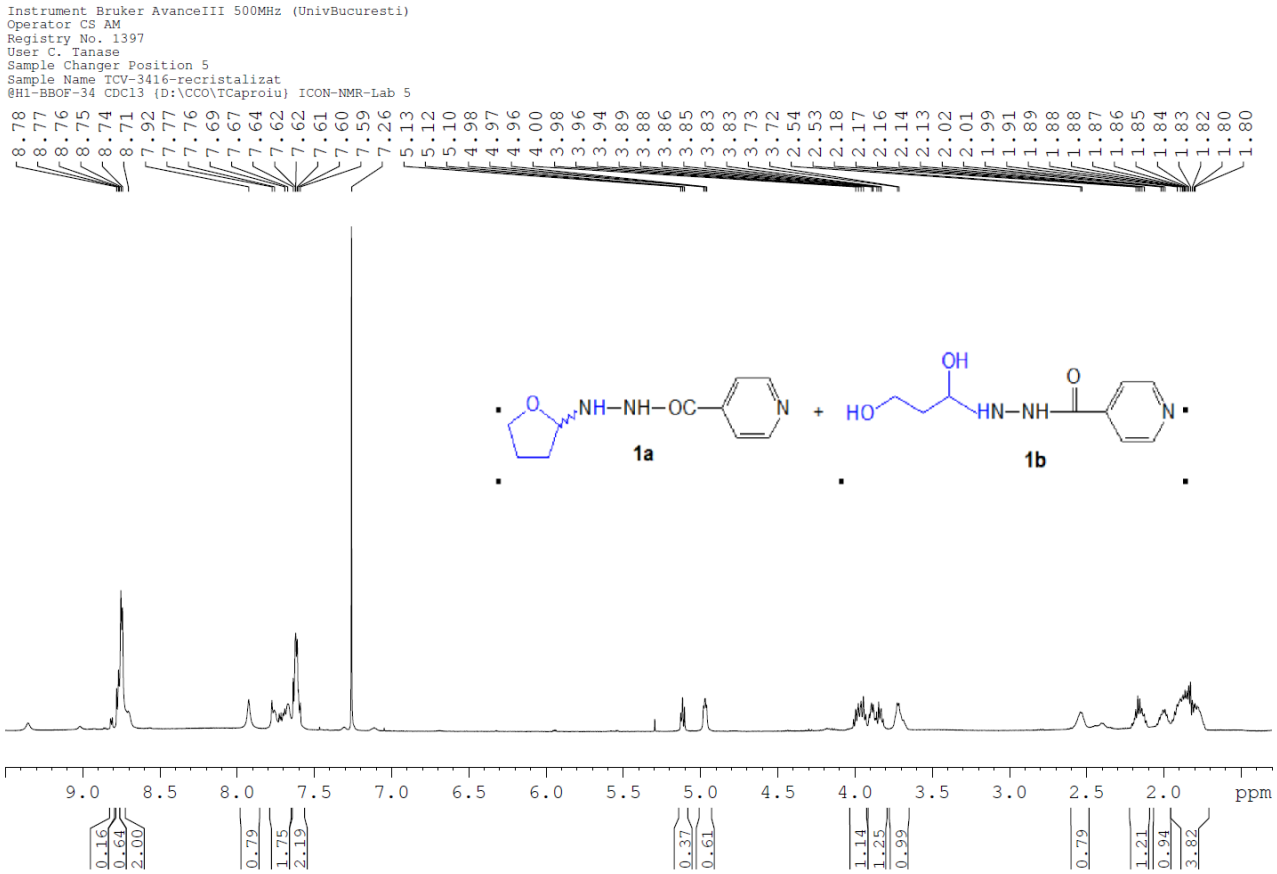
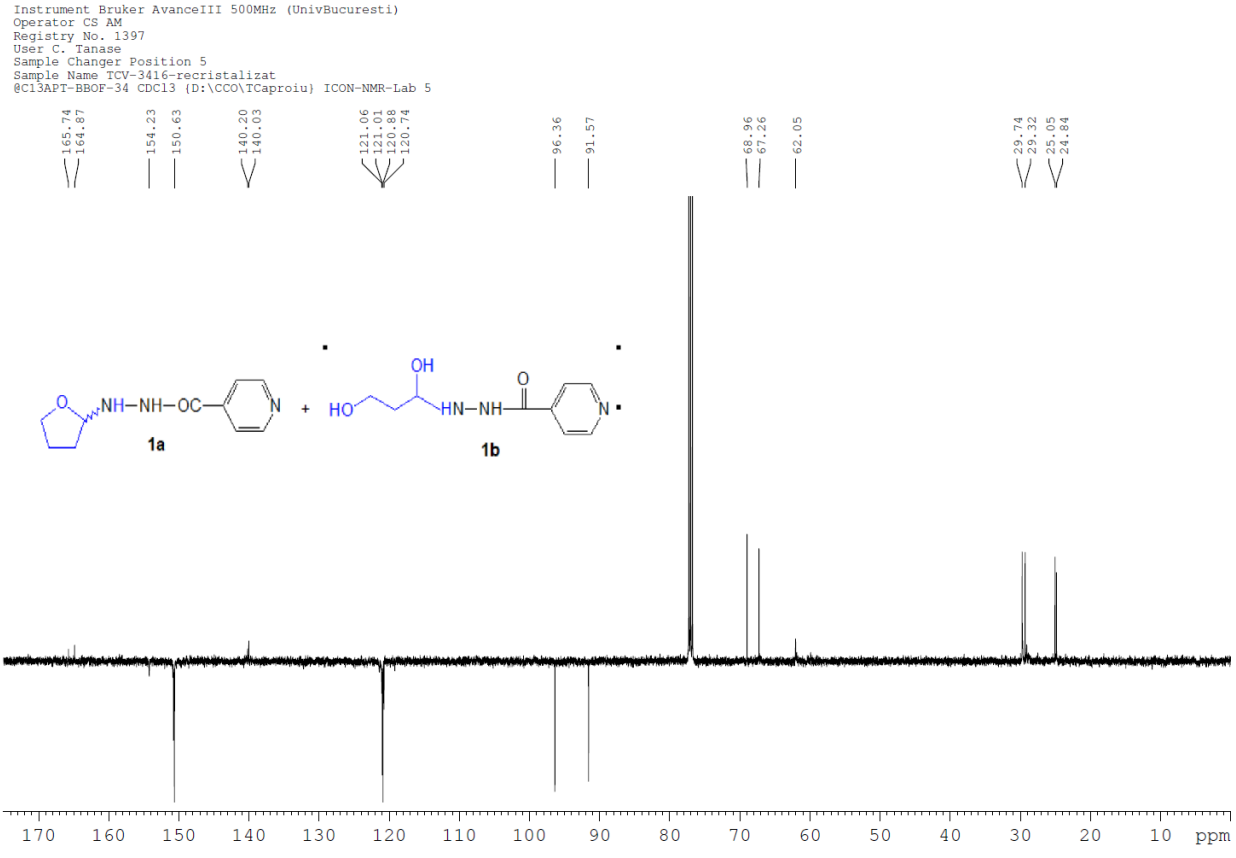
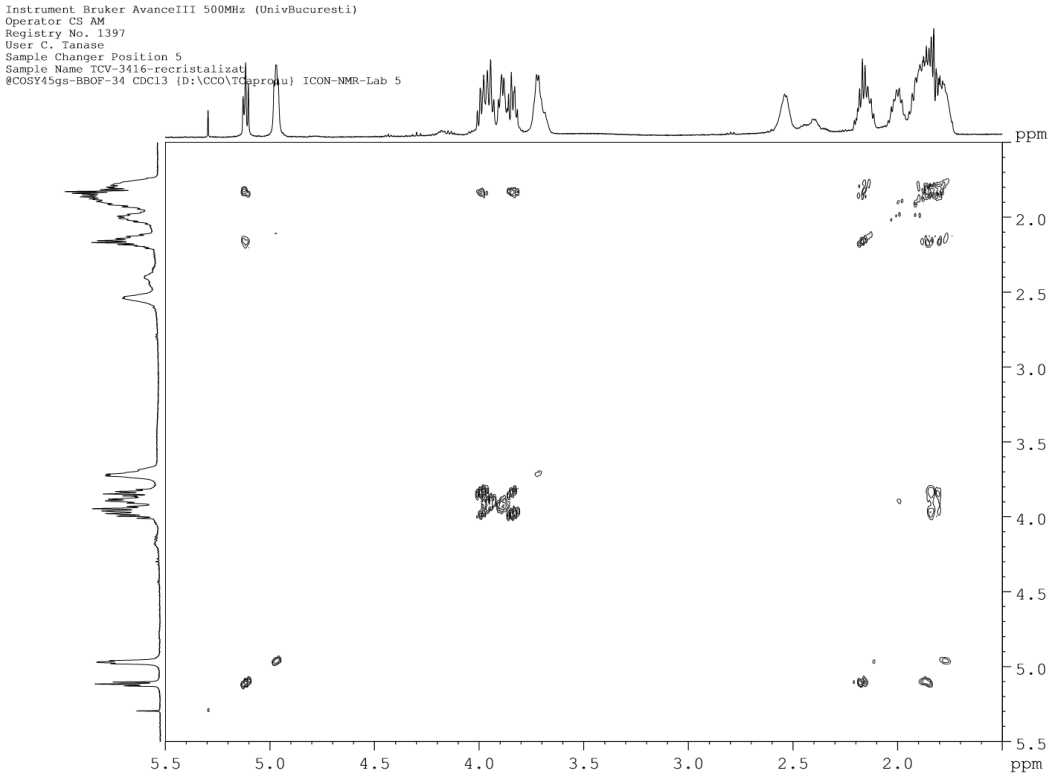
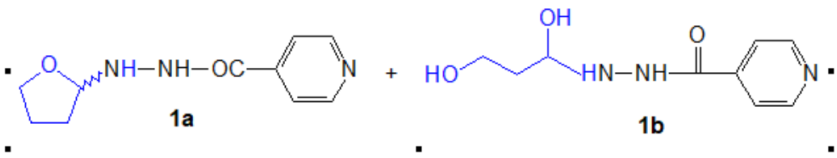
1. NMR Spectra of the compounds

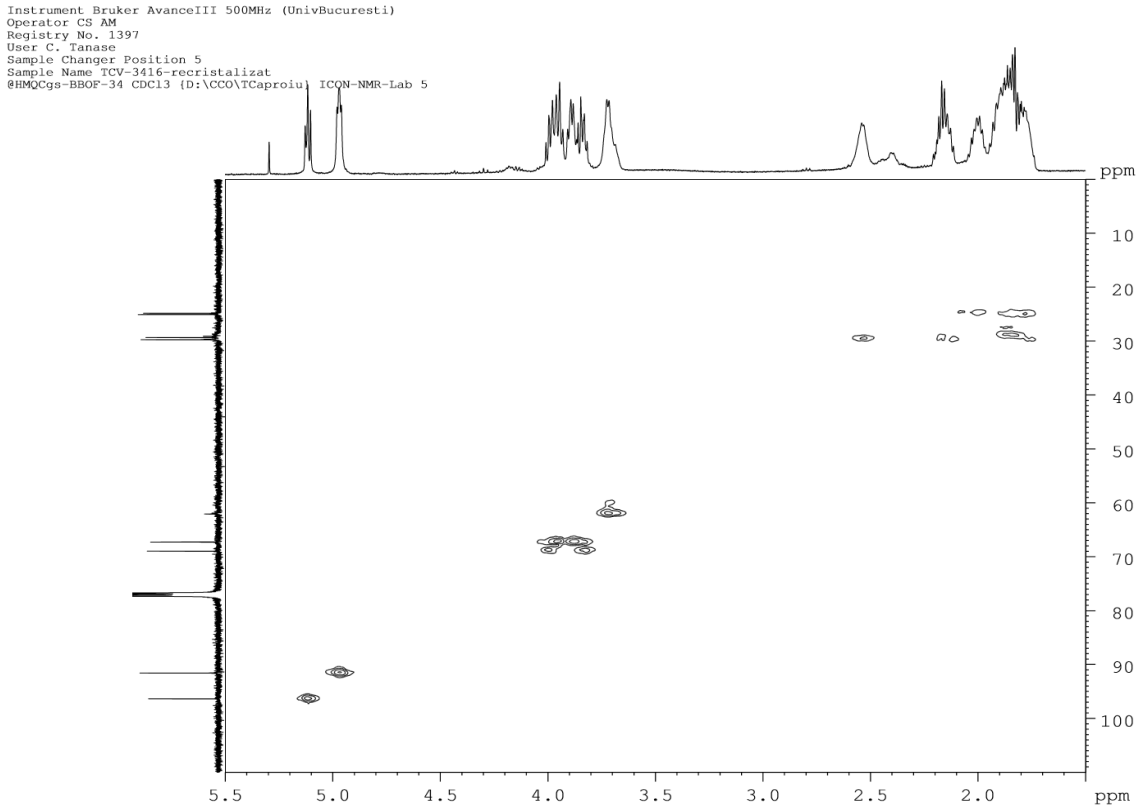
1.1. ^{1}H, ^{13}C, COSY and HETCOR-NMR spectra in $CDCl_3$ of the crystallized compound **1** isolated by LPC of a crude product obtained by reaction of INH with THF[X] in example 1.1.



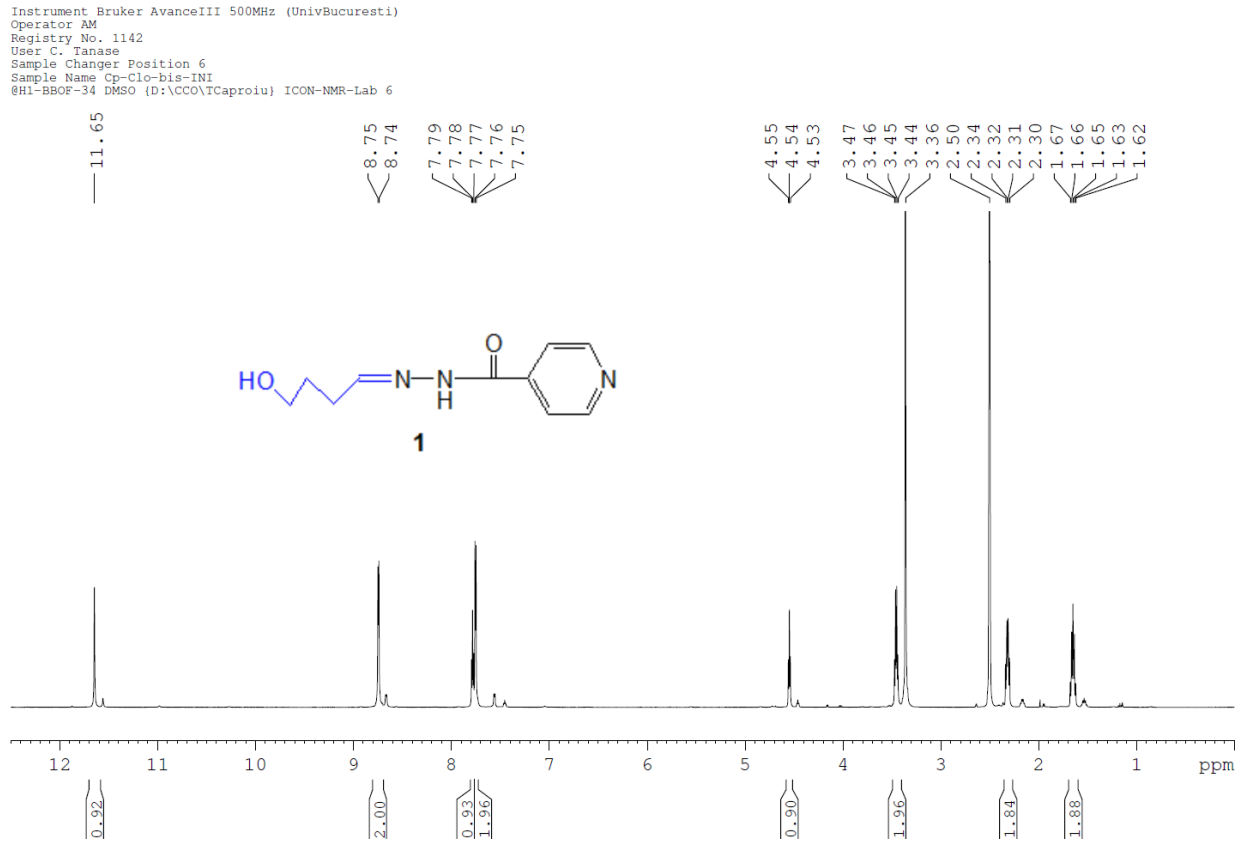


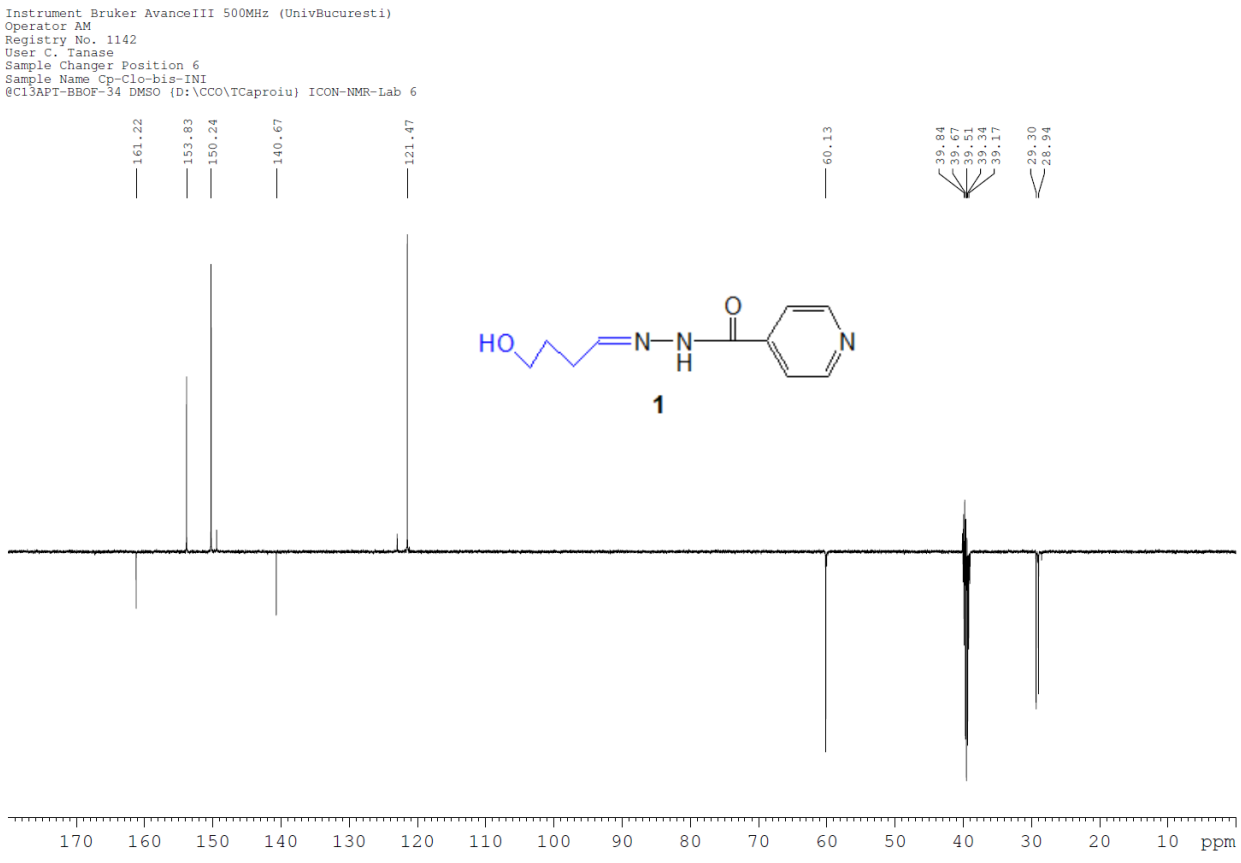

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1397
User C. Tanase
Sample Changer Position 5
Sample Name TCV-3416-recristalizat
@COSY45gs-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 5
ppm
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

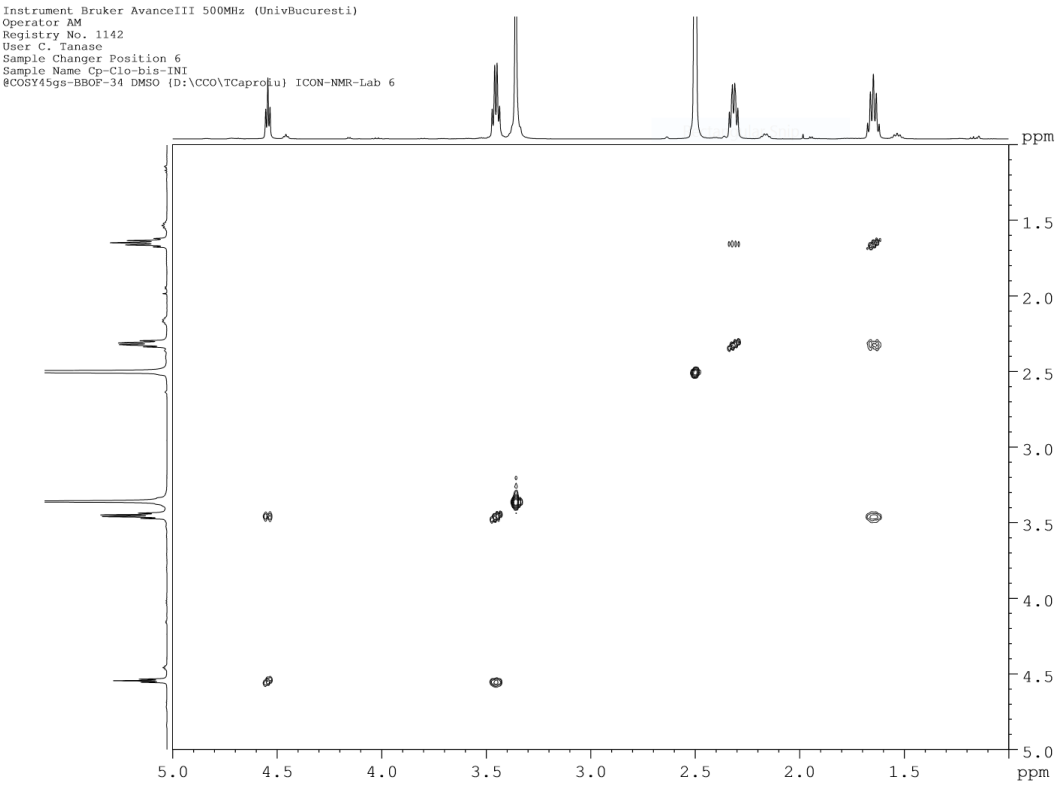

O
NH—NH—OC
N
1a
+
OH
HO
HN—NH
O
N
1b

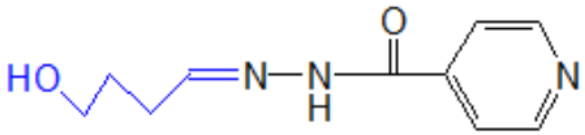

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1397
User C. Tanase
Sample Changer Position 5
Sample Name TCV-3416-recristalizat
@HMQCgs-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 5
ppm
10
20
30
40
50
60
70
80
90
100
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

1.2. ^{1}H, ^{13}C, COSY and HETCOR-NMR spectra in dry DMSO of the compound **1** (coded: Cp-Clo-bis-INI) isolated by LPC of a crude product obtained by reaction of INH with a cyclopentane aldehyde in THF[X]

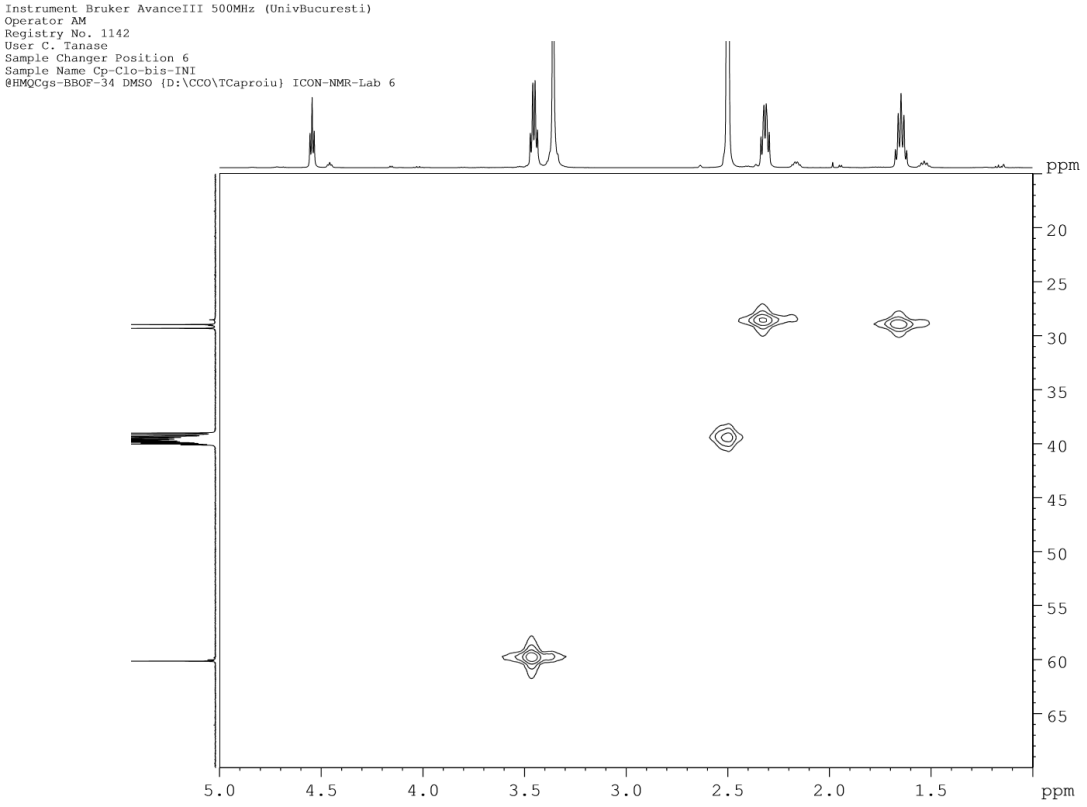


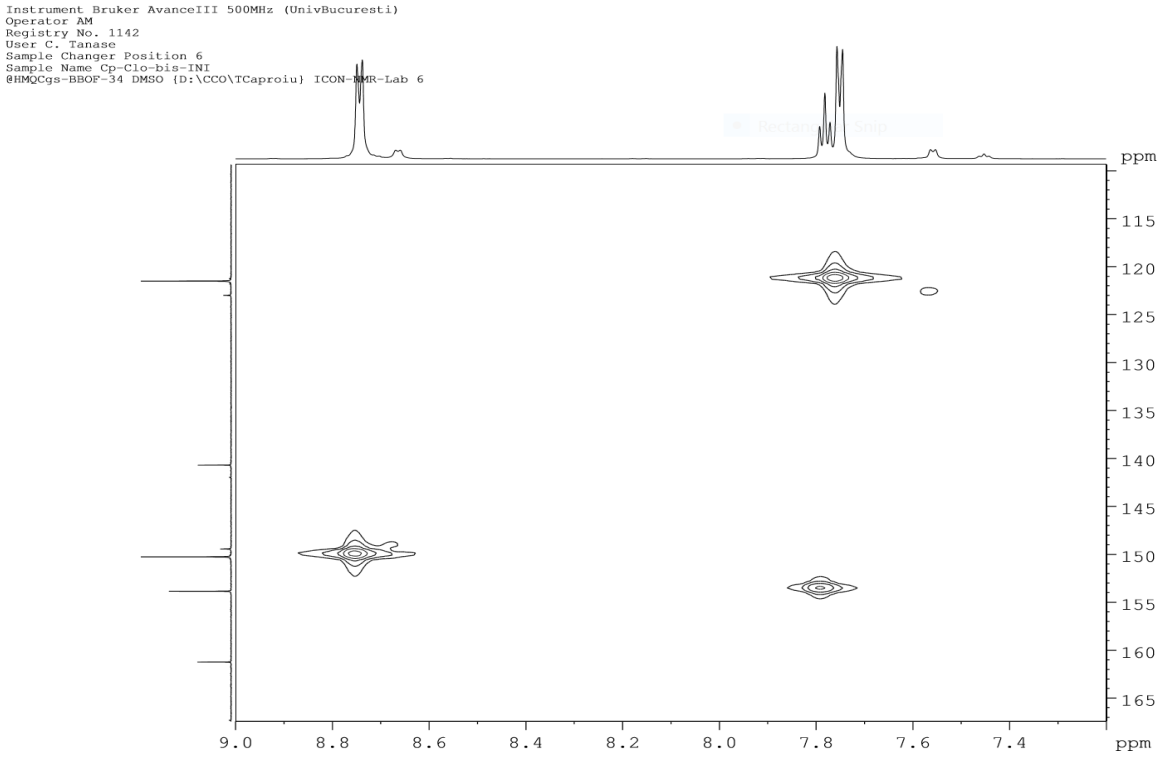



Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator AM
Registry No. 1142
User C. Tanase
Sample Changer Position 6
Sample Name Cp-Clo-bis-INI
@COSY45gs-BBOF-34 DMSO {D:\CCO\TCaproiu} ICON-NMR-Lab 6
ppm
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

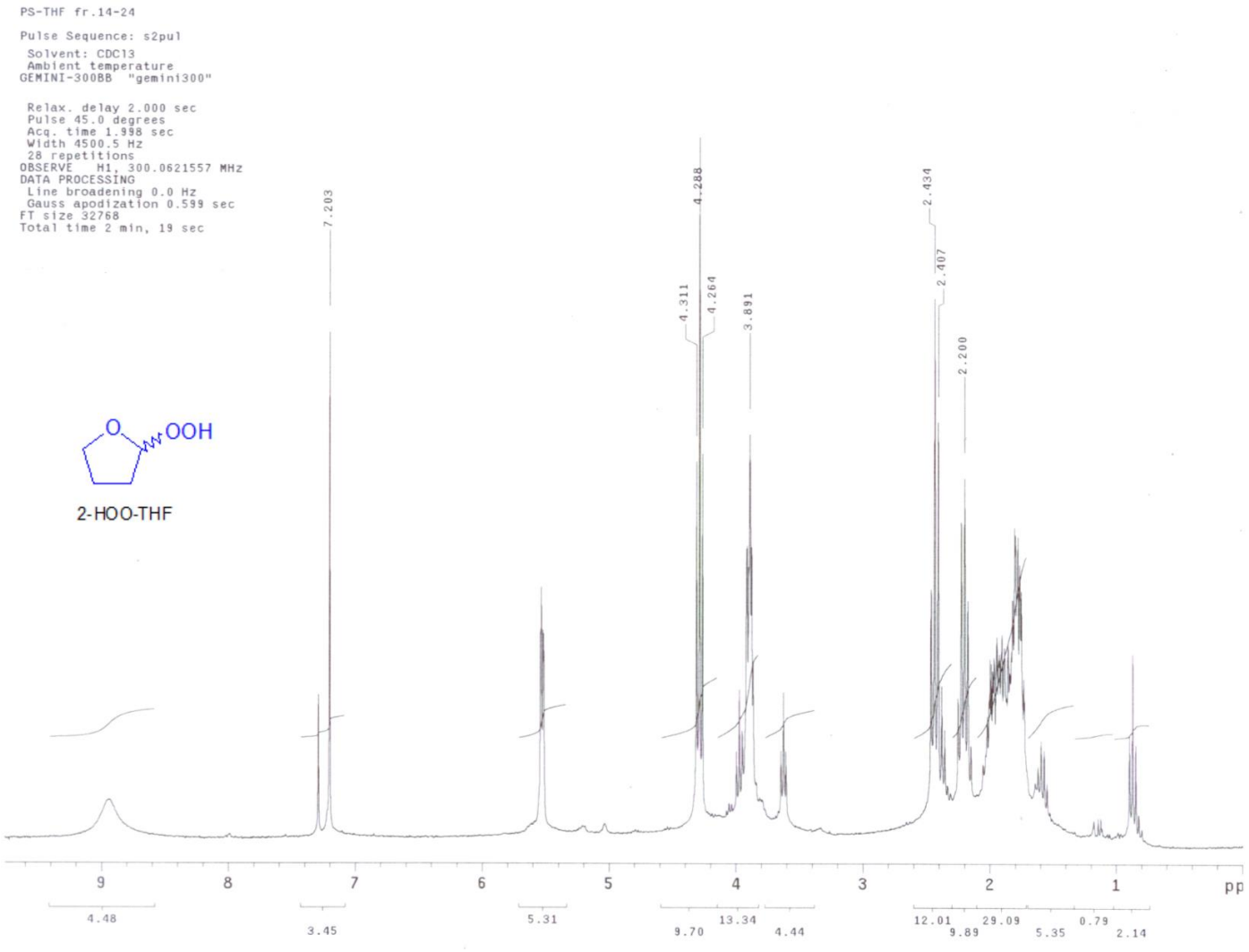

HO
N
N
H
O
N

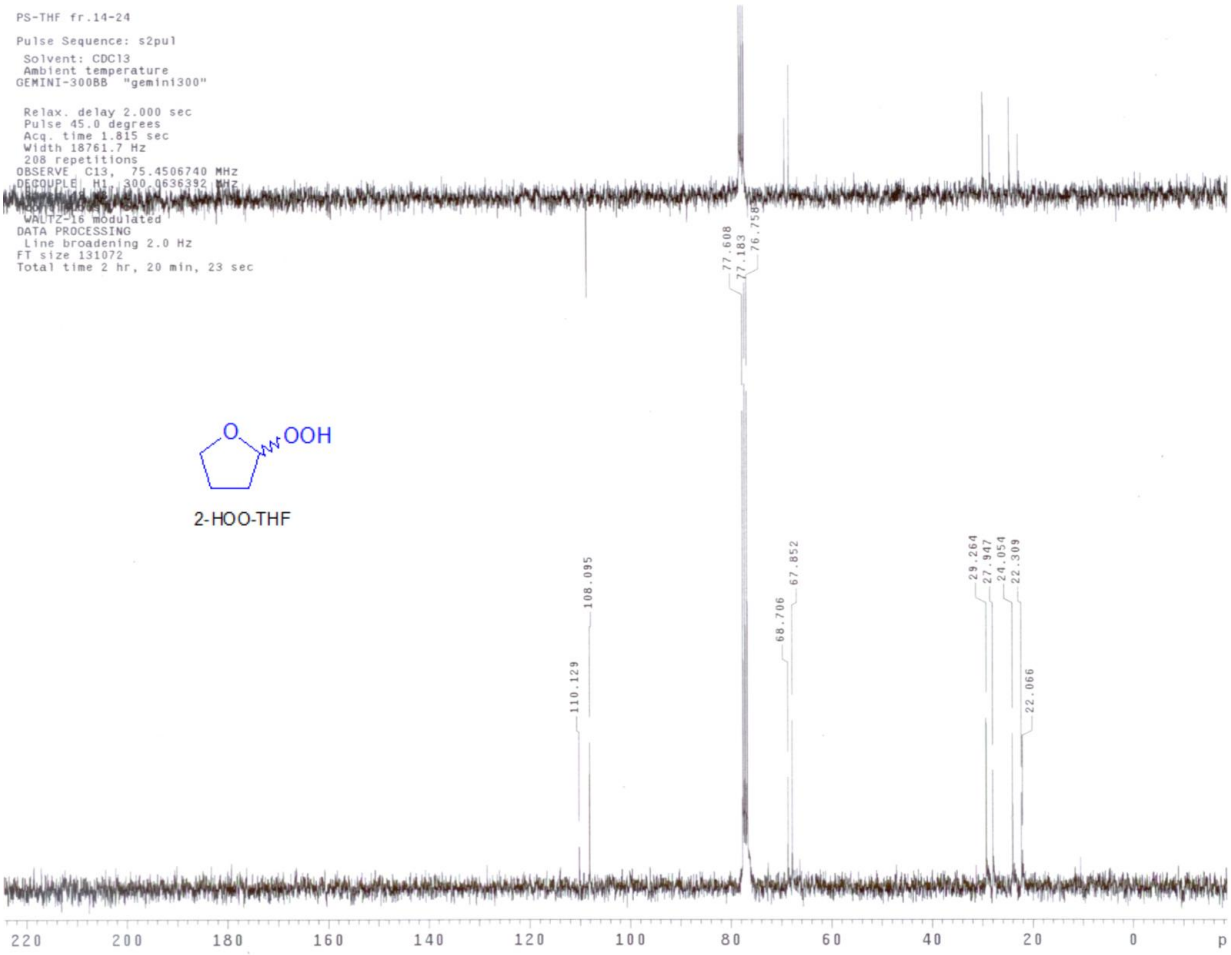
1


Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator AM
Registry No. 1142
User C. Tanase
Sample Changer Position 6
Sample Name Cp-Clo-bis-INI
@HMQCgs-BBOF-34 DMSO {D:\CCO\TCaproiu} ICON-NMR-Lab 6
ppm
20
25
30
35
40
45
50
55
60
65
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

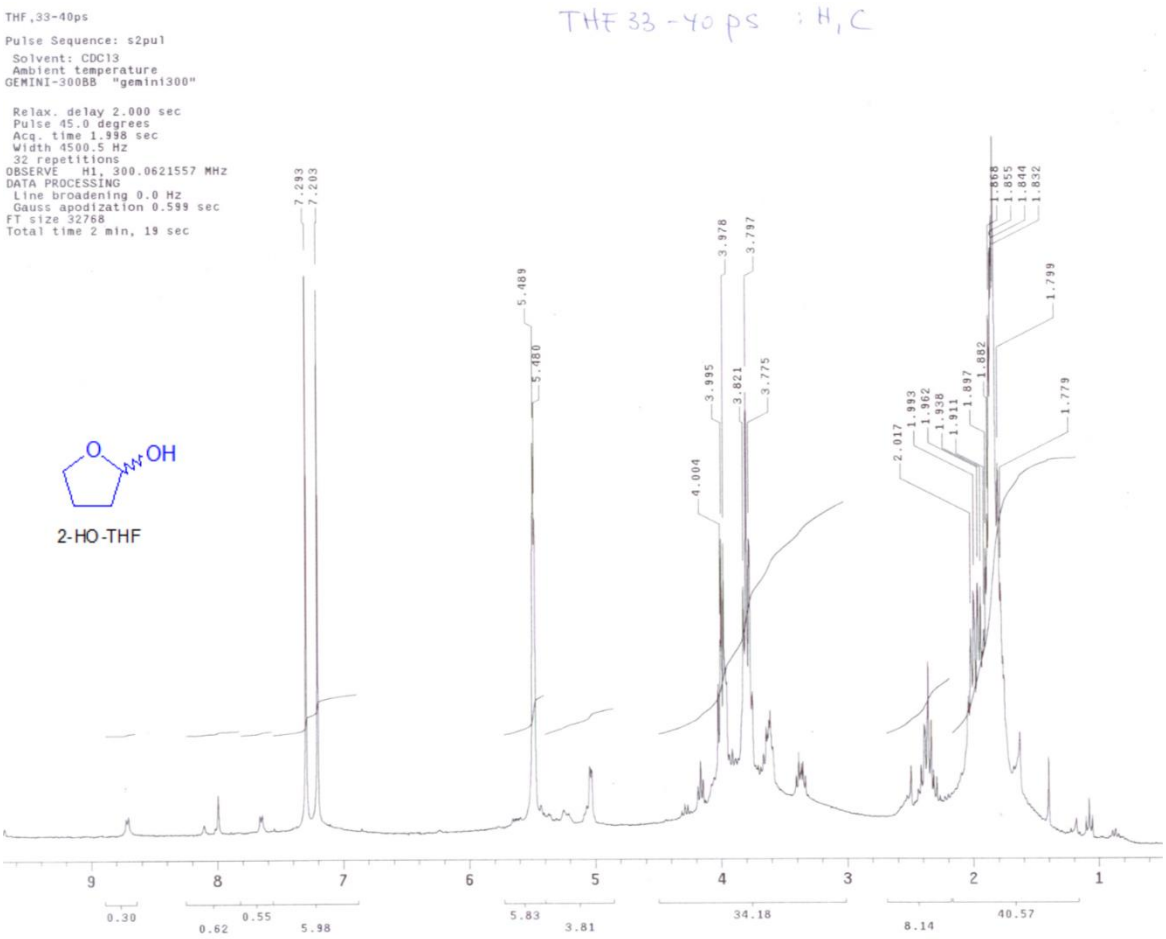


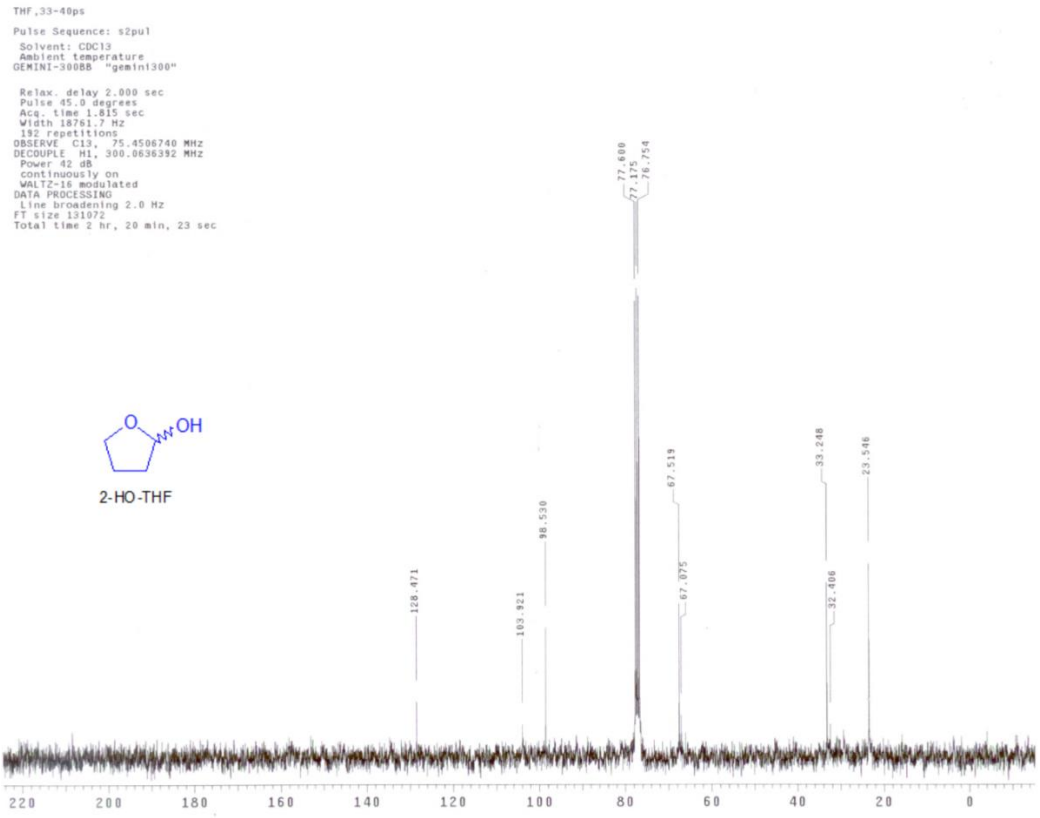
1.3. ^{1}H and ^{13}C-NMR spectra in $CDCl_3$ of 2-HOO-THF (fr. 14-24) isolated by LPC of an aliquot of THF[x]



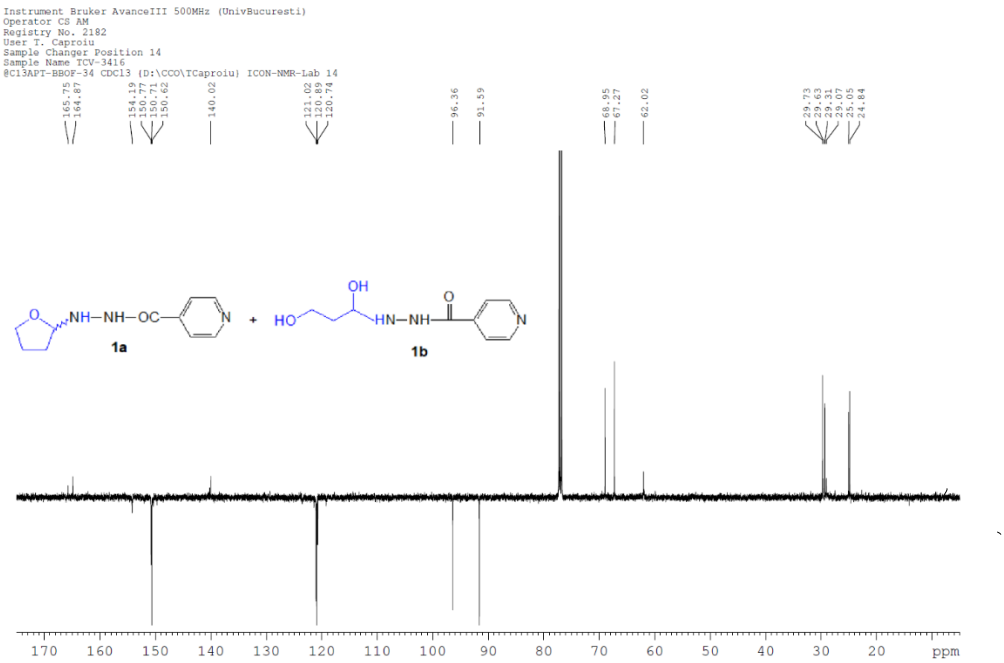


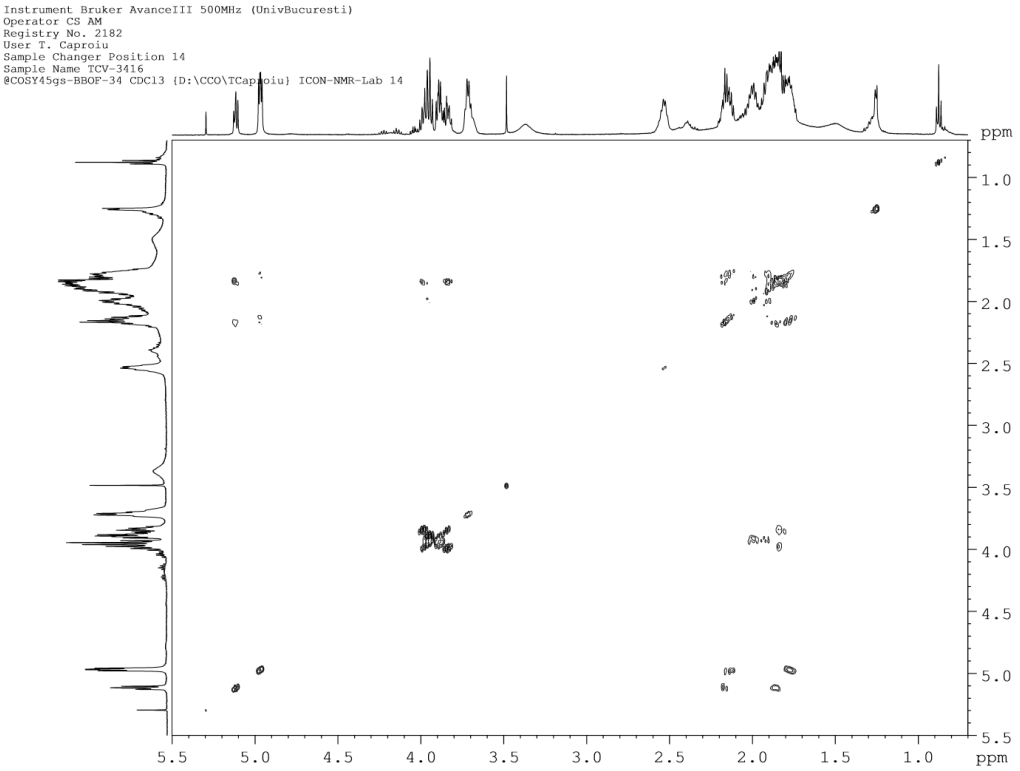
1.4 ^{1}H and ^{13}C-NMR spectra in $CDCl_3$ of the 2-HO-THF (fr. 33-44) isolated by LPC of an aliquot of THF[x]

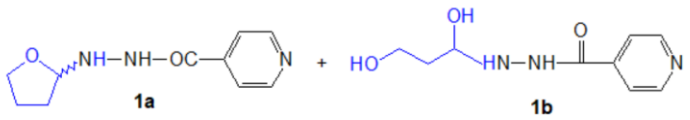


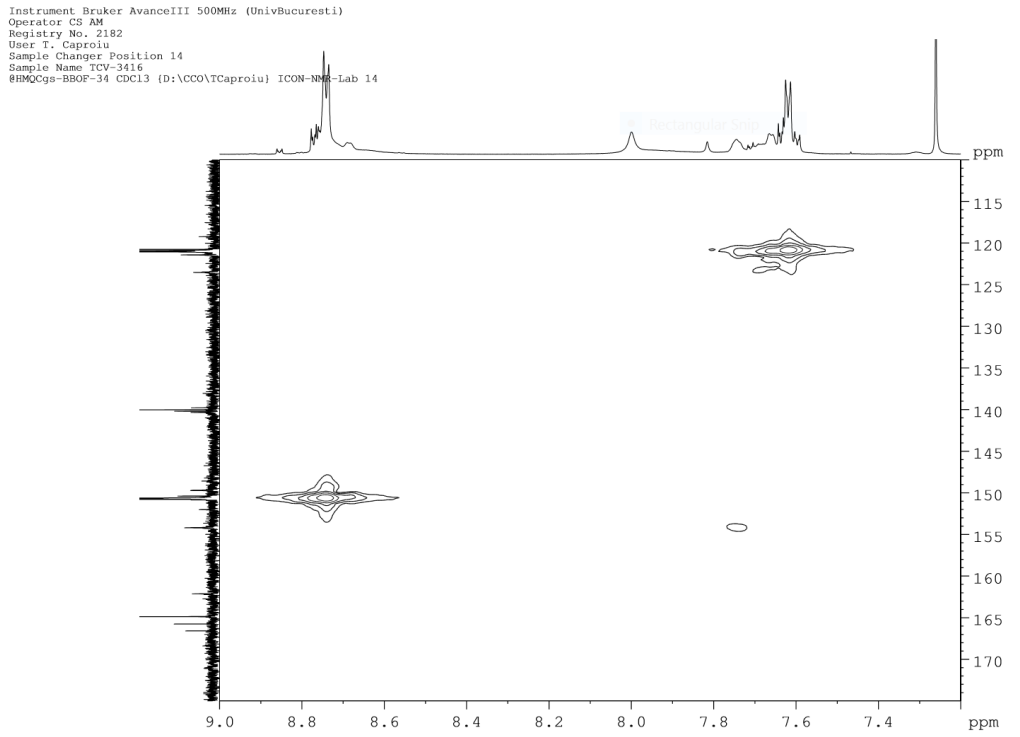


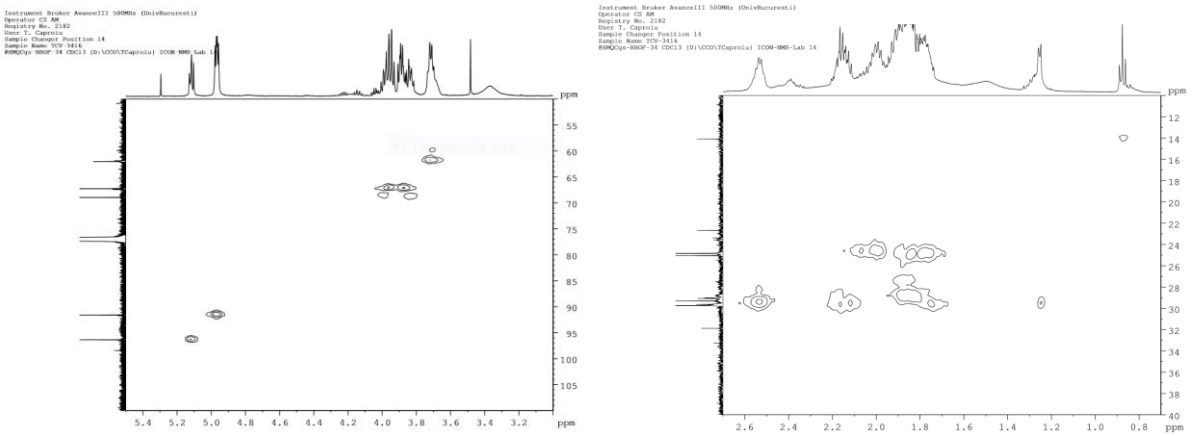
1.5. ^{13}C, COSY (Aliphatic and aromatic) and HETCOR (Aliphatic and aromatic) NMR spectra in $CDCl_3$ of the crystallized compound **1** isolated by LPC of a crude product obtained by reaction of INH with THF[X]

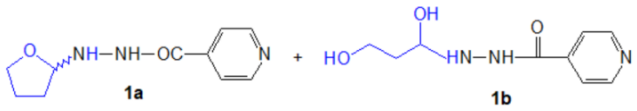



Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 2182
User T. Caproiu
Sample Changer Position 14
Sample Name TCV-3416
@COSY45gs-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 14
ppm
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

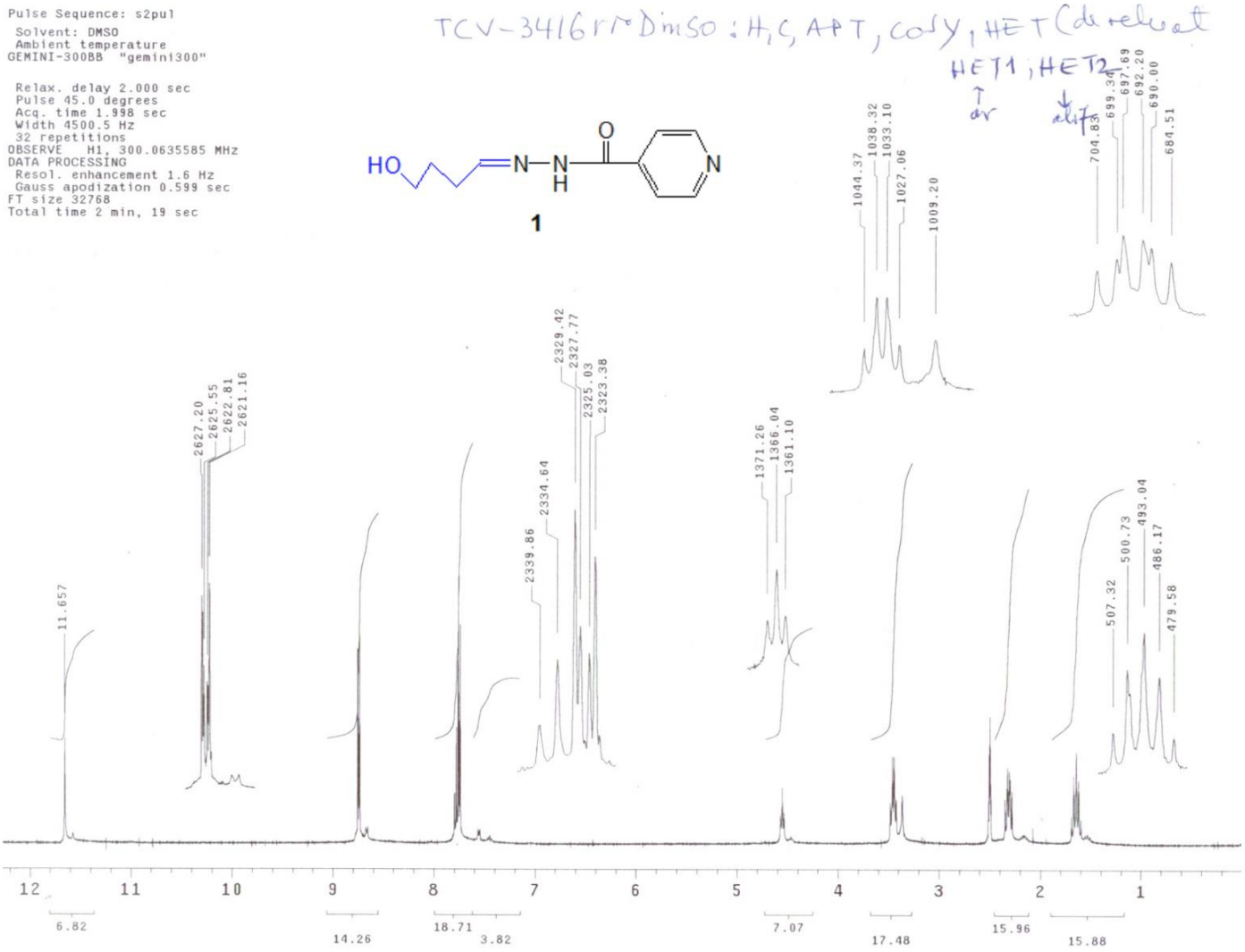

O
NH—NH—OC
N
1a
+
OH
HO
HN—NH
O
N
1b

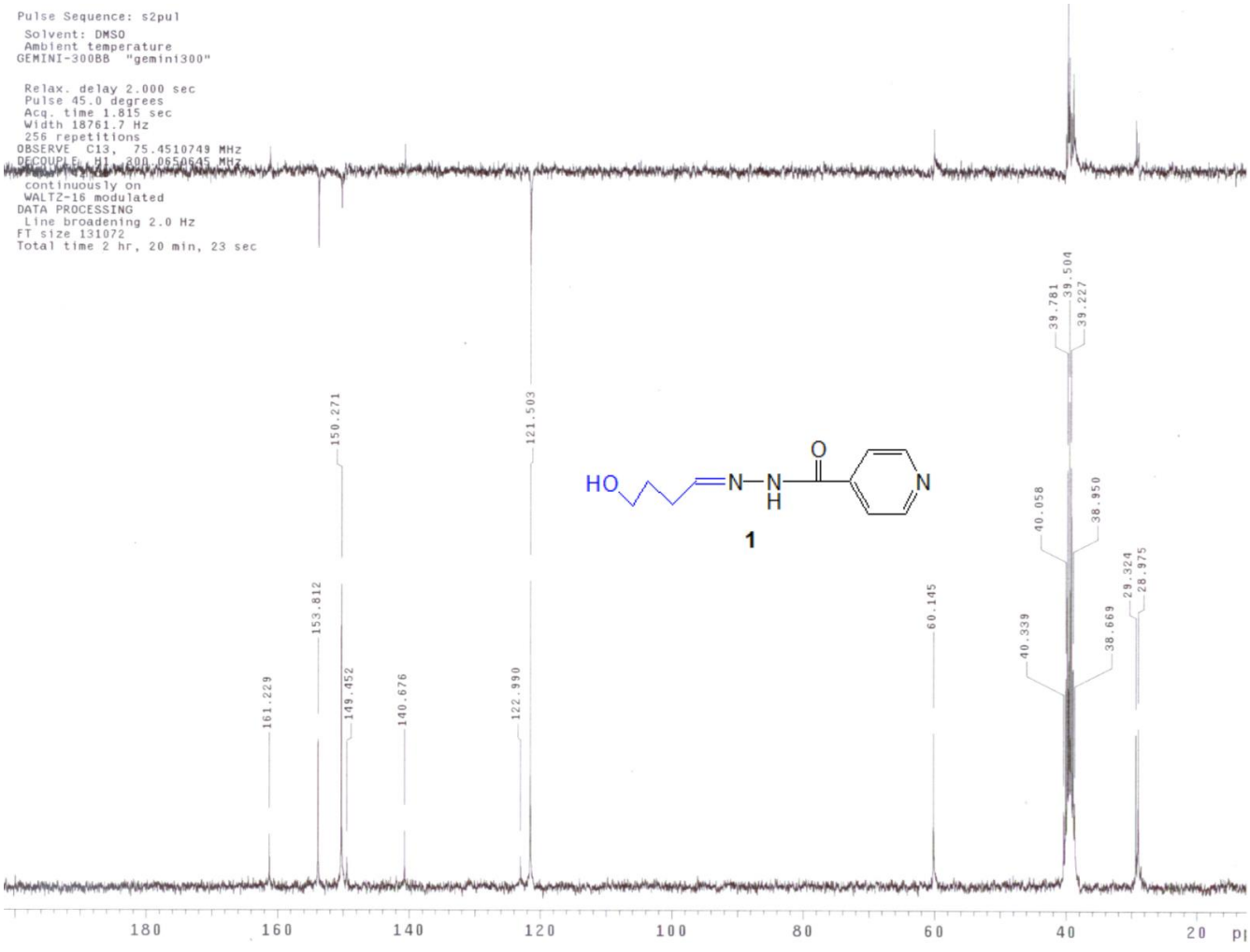

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 2182
User T. Caproiu
Sample Changer Position 14
Sample Name TCV-3416
@HMQCgs-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 14
ppm
115
120
125
130
135
140
145
150
155
160
165
170
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm

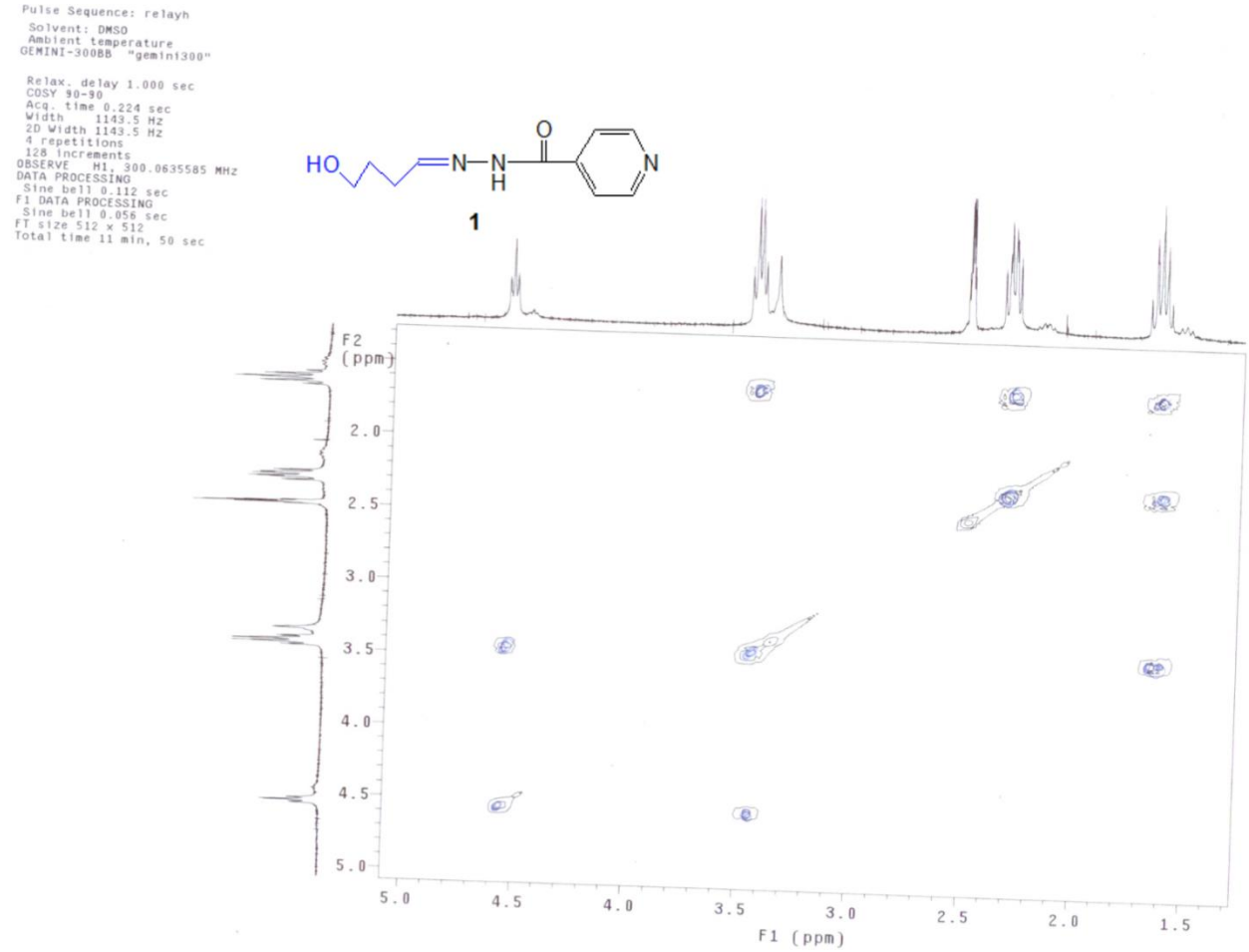


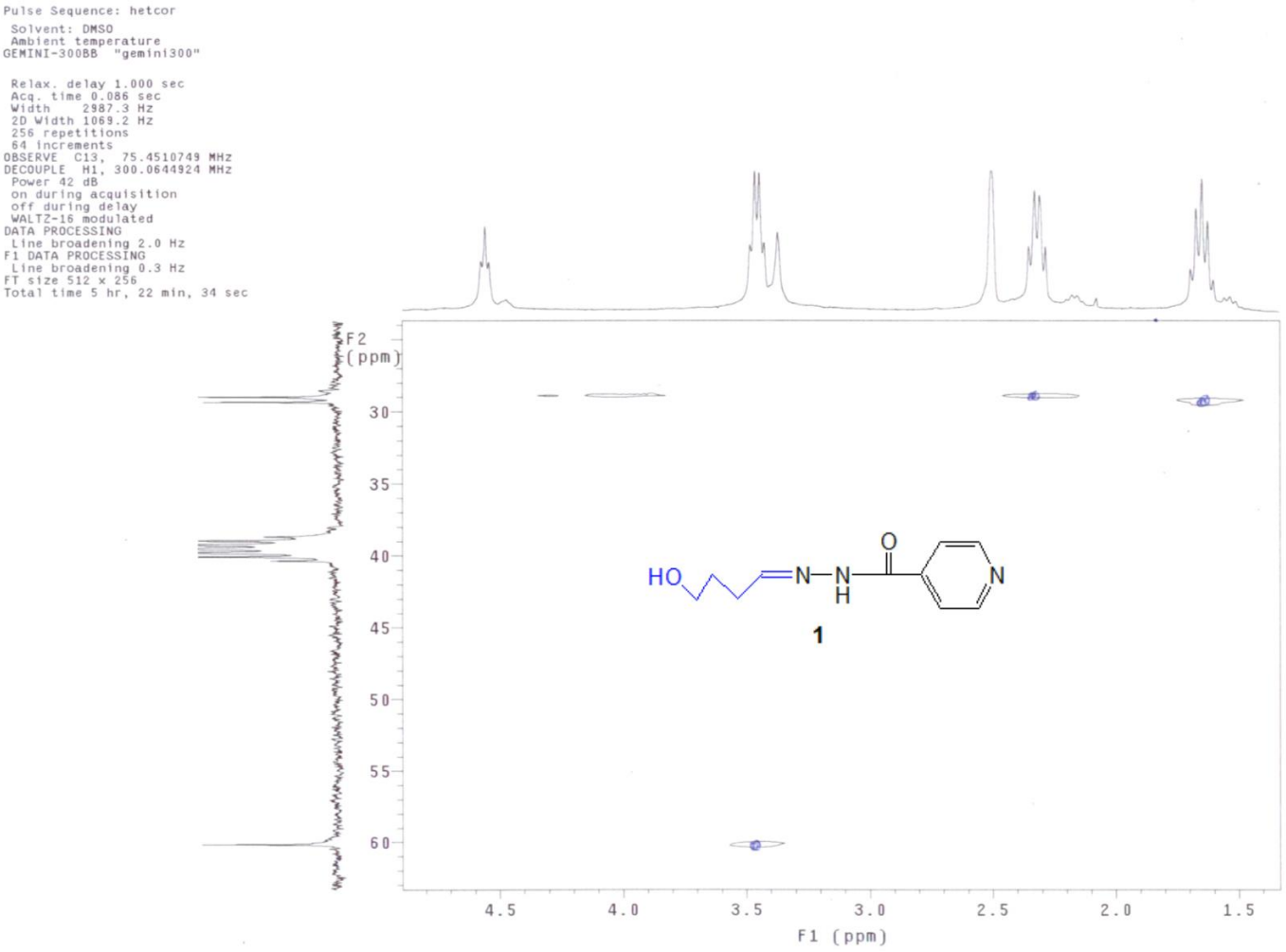


1.6. ^{1}H, ^{13}C, COSY and HETCOR-NMR spectra in DMSO of *the same crystallized compound* **1** isolated by LPC of a crude product obtained by reaction of INH with THF[X]

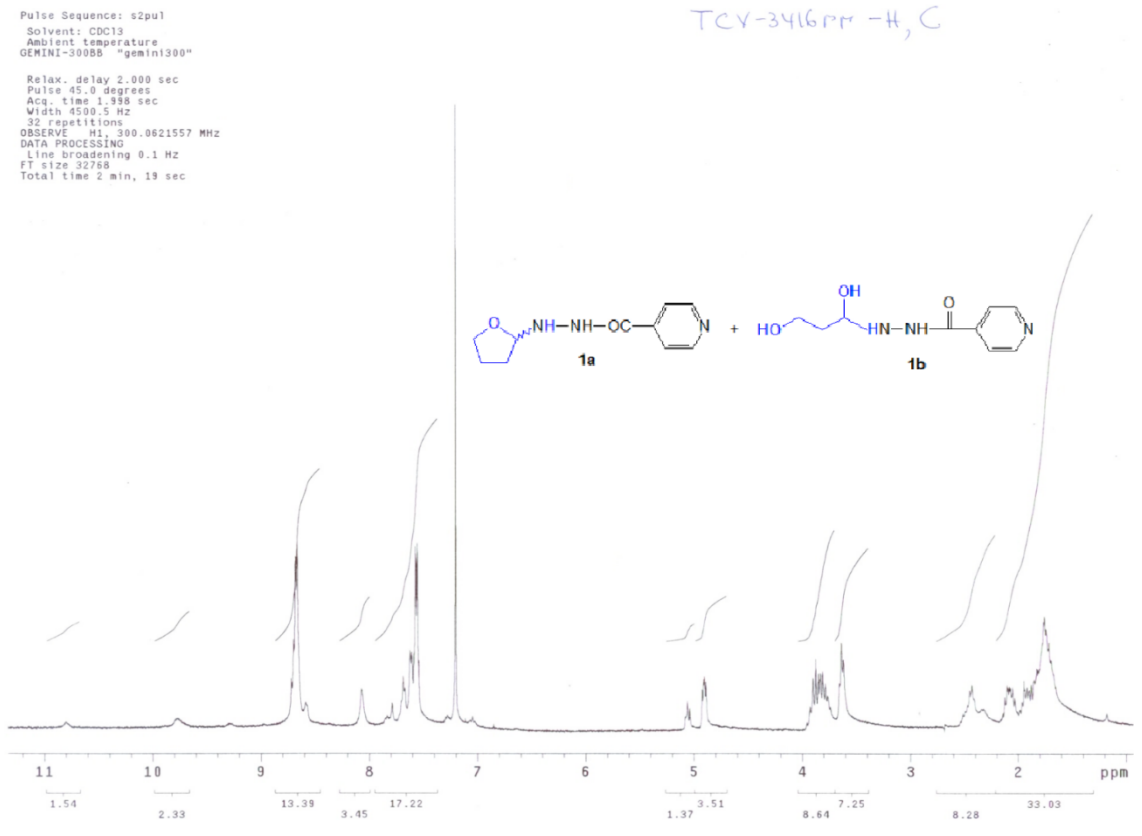


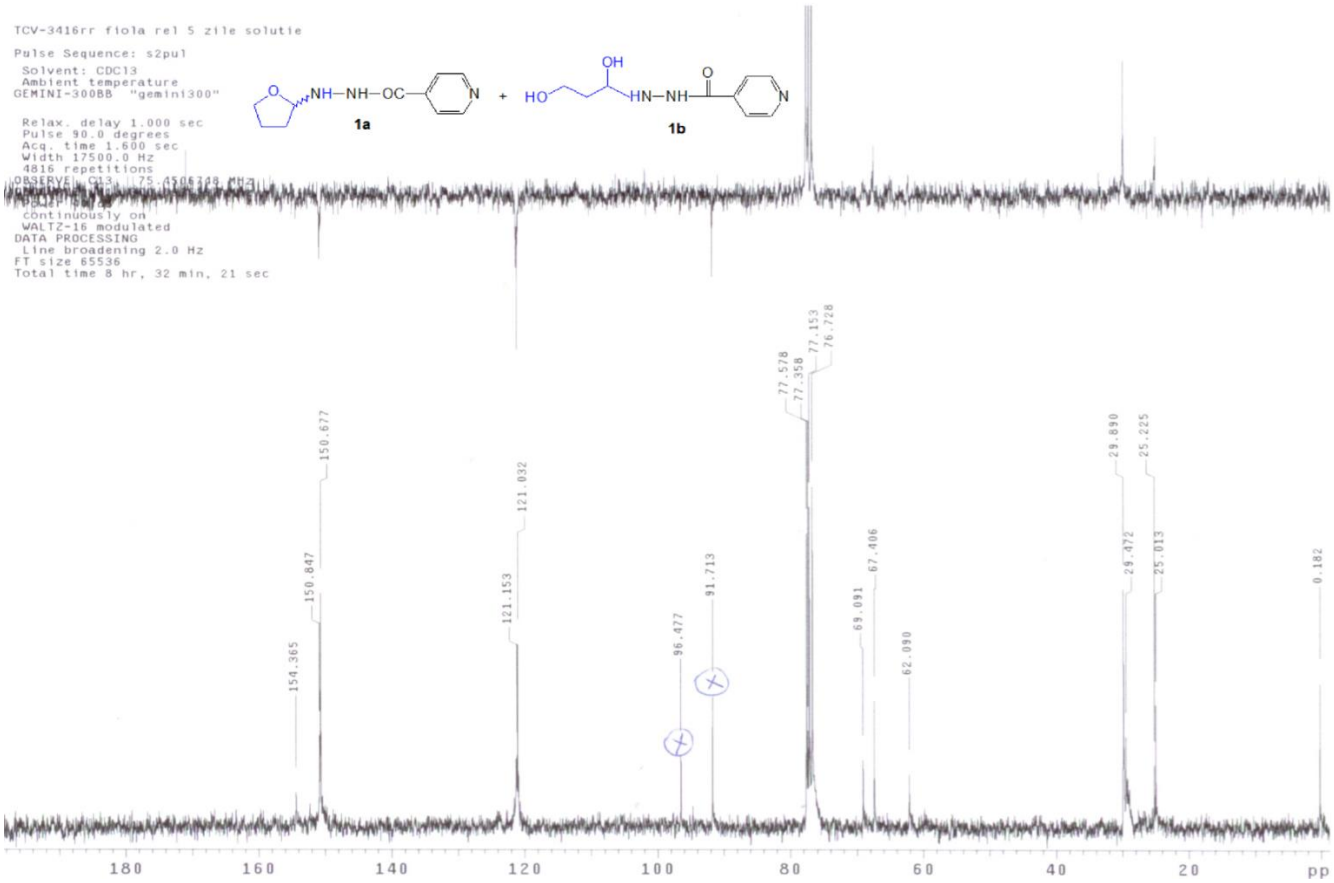

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
GEMINI-300BB "gemini300"
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
256 repetitions
OBSERVE C13, 75.4510749 MHz
DECOUPLE H1, 300.0650645 MHz
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 20 min, 23 sec
150.271
121.503
153.812
149.452
140.676
122.990
161.229
60.145
40.339
39.781
39.504
39.227
40.058
38.950
38.669
29.324
28.975
HO
N
N
H
O
N
1
180
160
140
120
100
80
60
40
20
pp


Pulse Sequence: relayh
Solvent: DMSO
Ambient temperature
GEMINI-300BB "gemini300"
Relax. delay 1.000 sec
COSY 90-90
Acq. time 0.224 sec
Width 1143.5 Hz
2D Width 1143.5 Hz
4 repetitions
128 increments
OBSERVE H1, 300.0635585 MHz
DATA PROCESSING
Sine bell 0.112 sec
F1 DATA PROCESSING
Sine bell 0.056 sec
FT size 512 x 512
Total time 11 min, 50 sec
HO
N
N
H
O
N
1
F2 (ppm)
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
F1 (ppm)

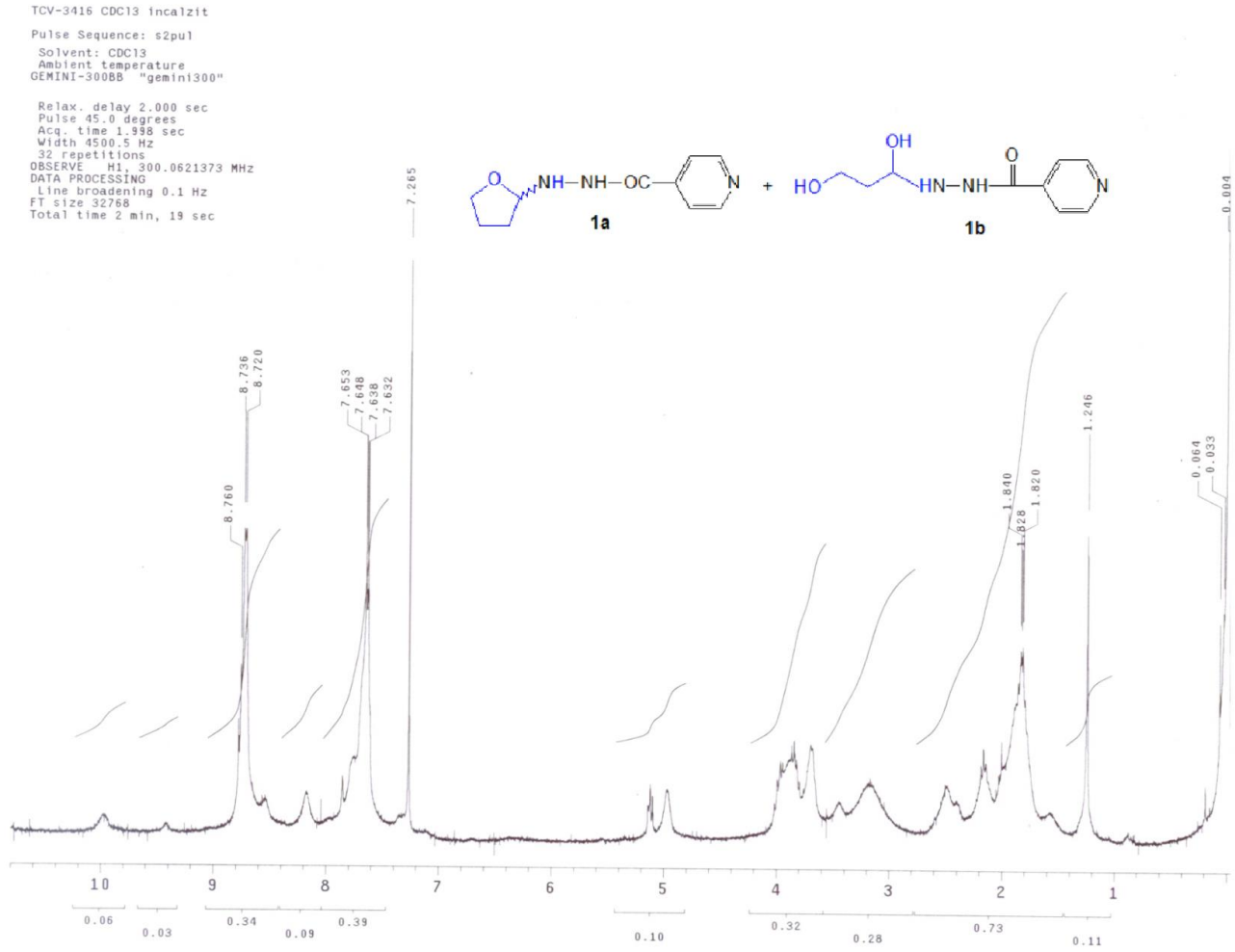


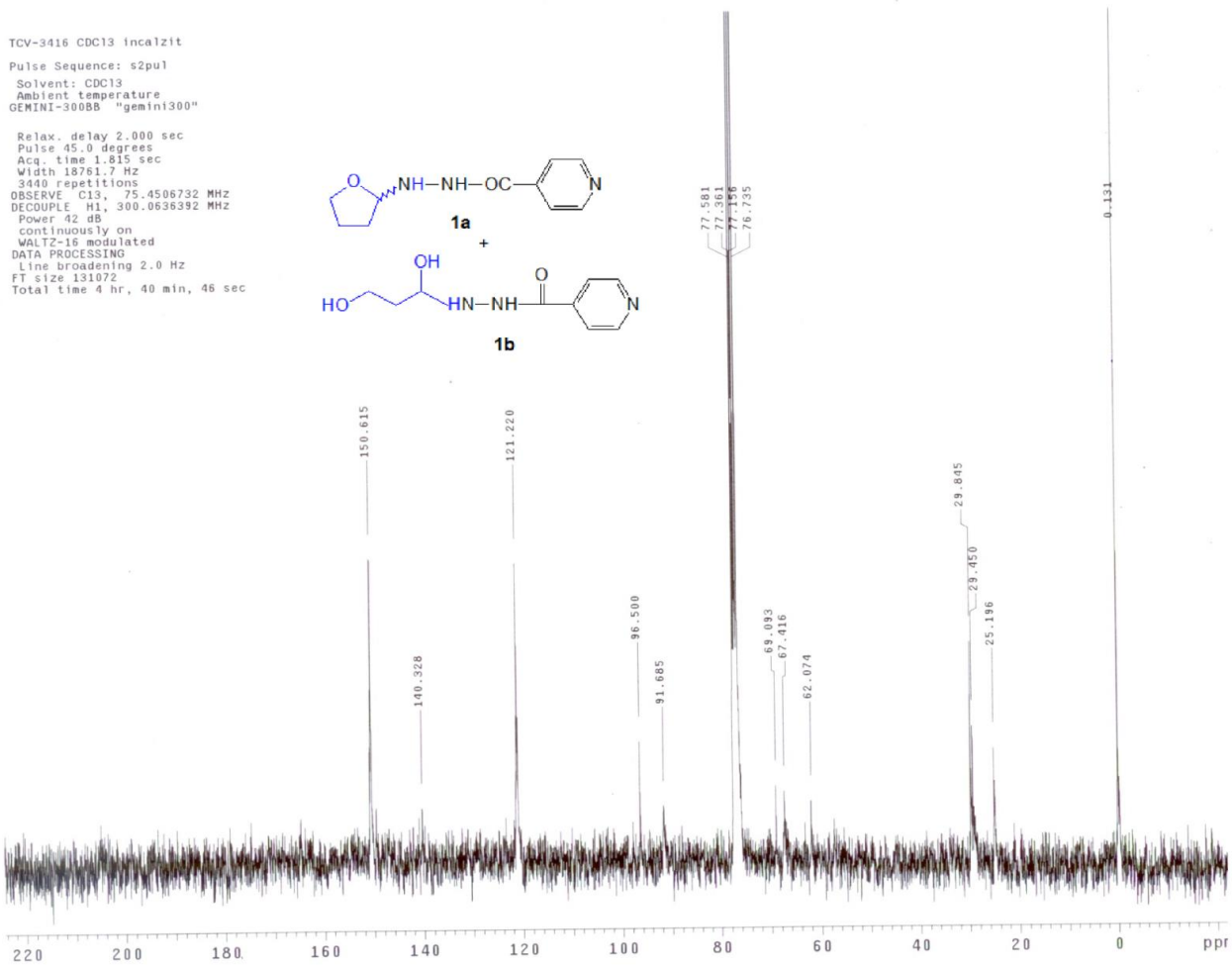
1.7. ^{1}H, ^{13}C (and then heating in tube) NMR spectra in $CDCl_3$ of *crystallized compound* **1** *directly from the crude product* of the reaction of INH with THF[X] reduced with triphenylphosphine



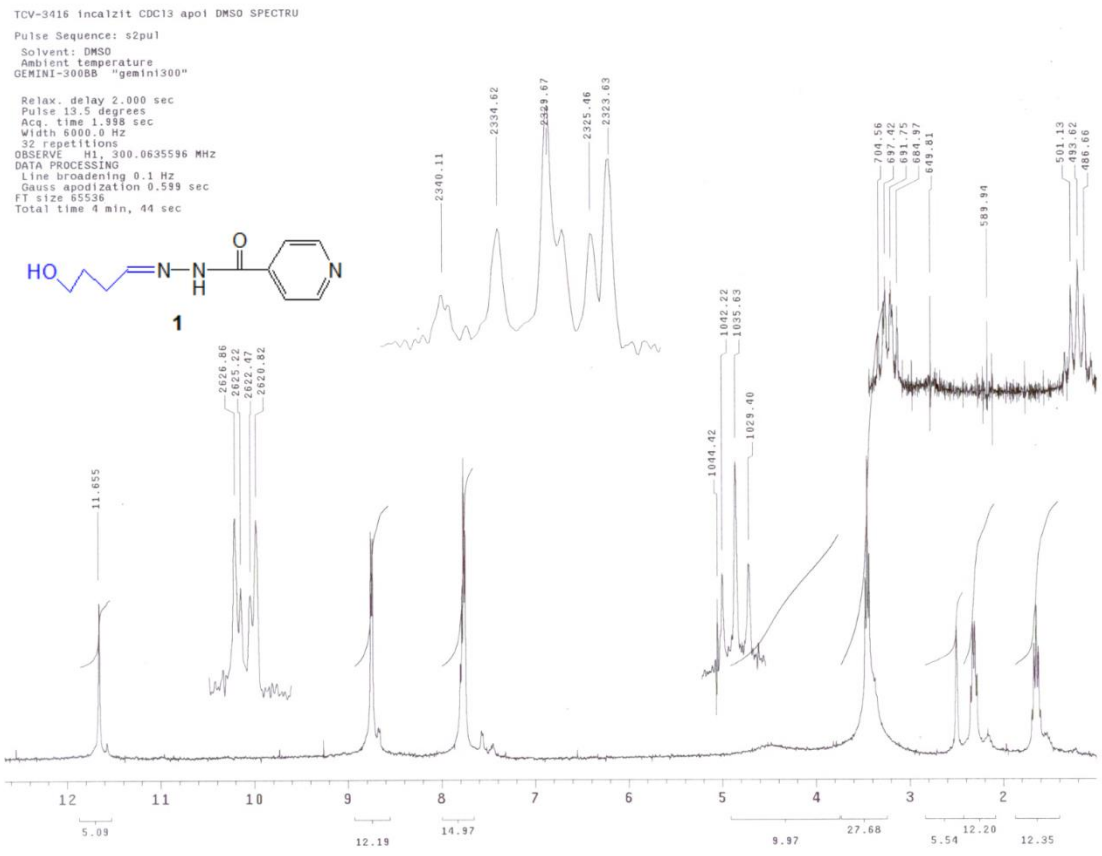


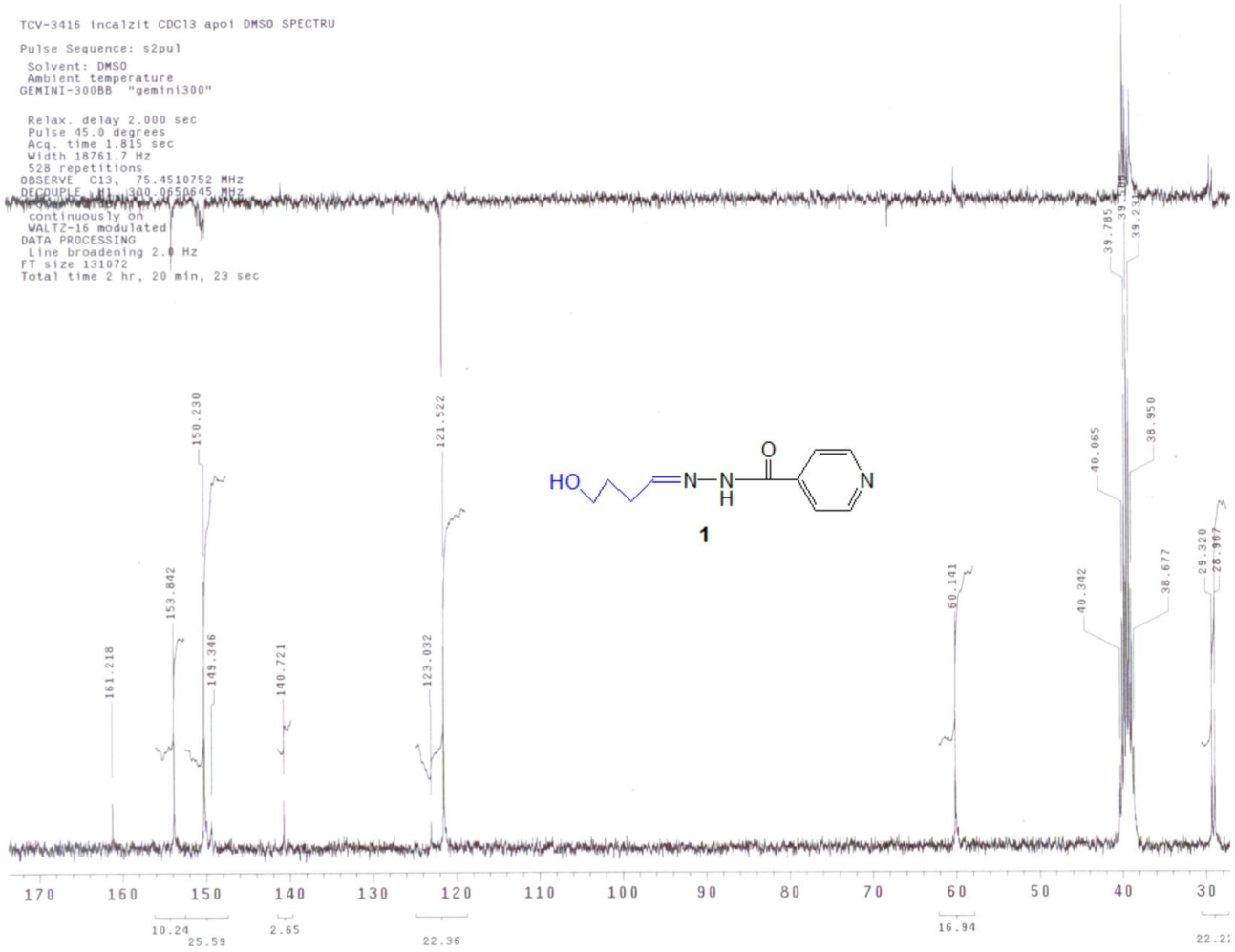
Heating in NMR tube





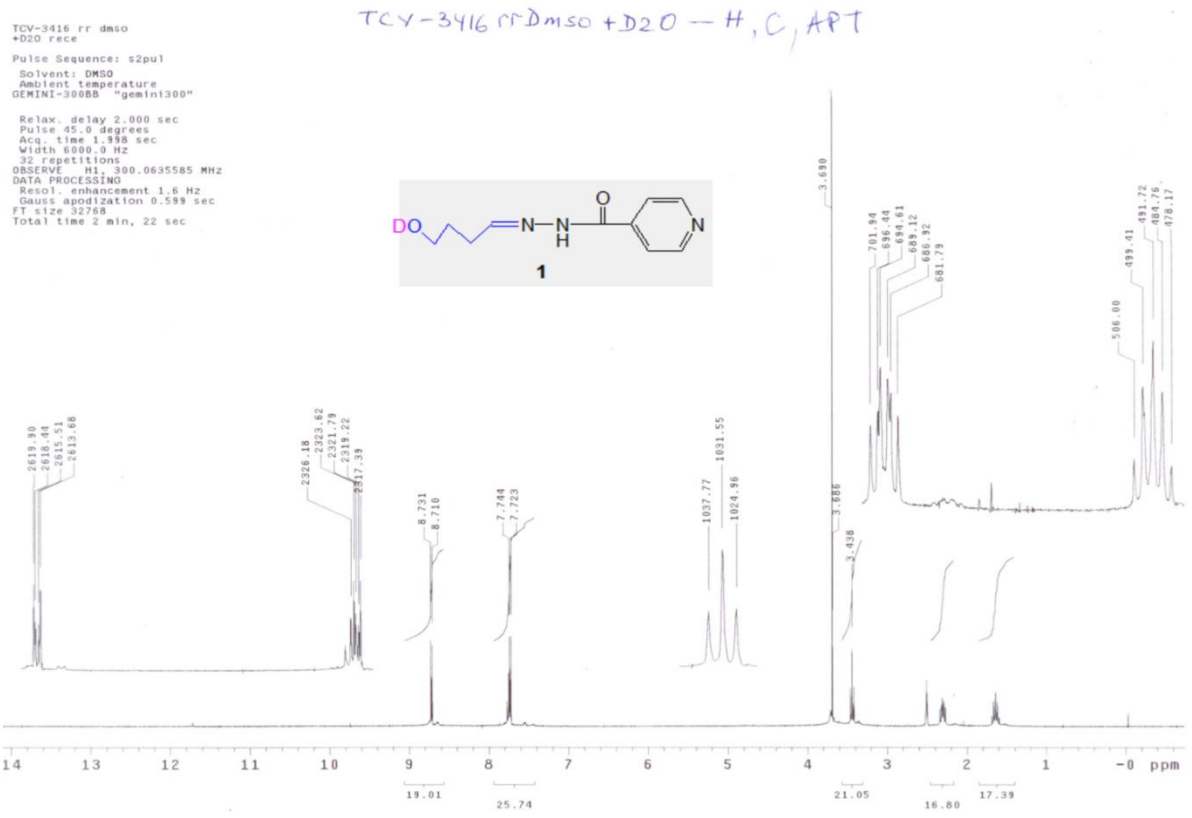
After heating, the solvent evaporated on the air, then spectra performed in DMSO

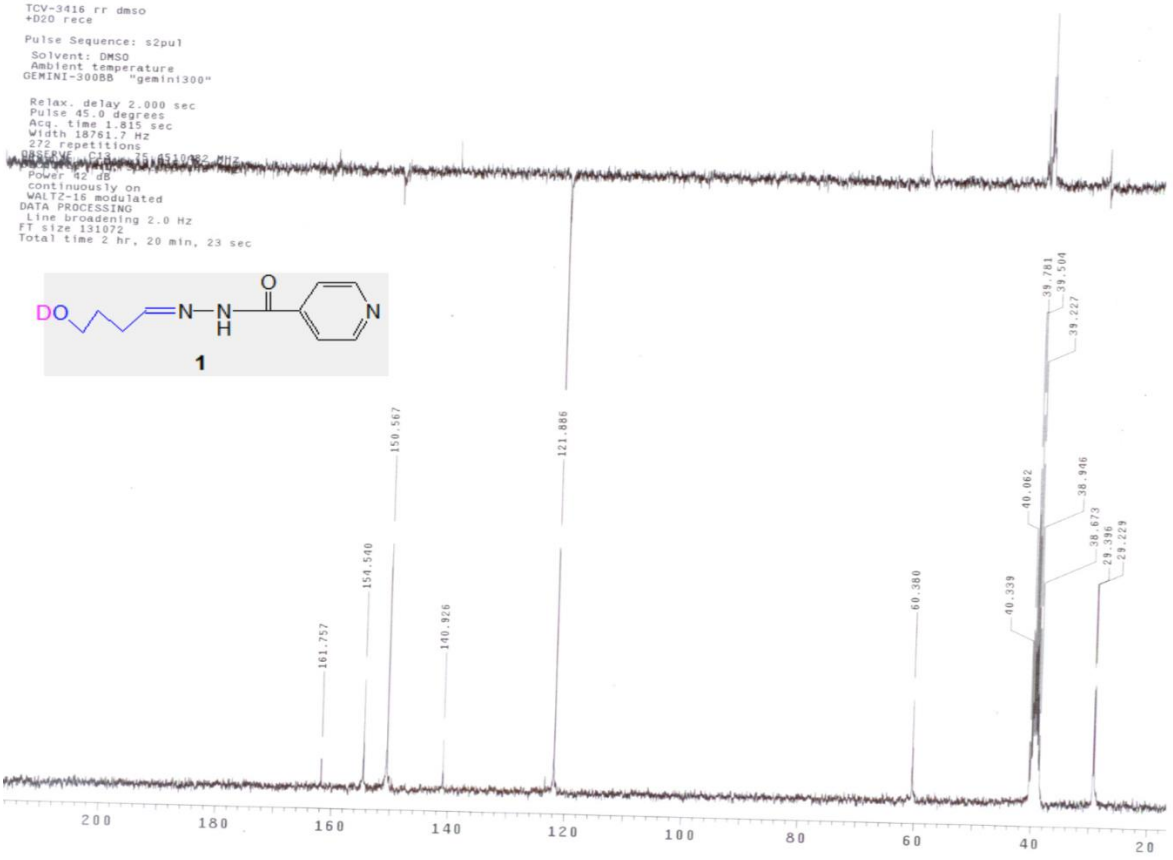


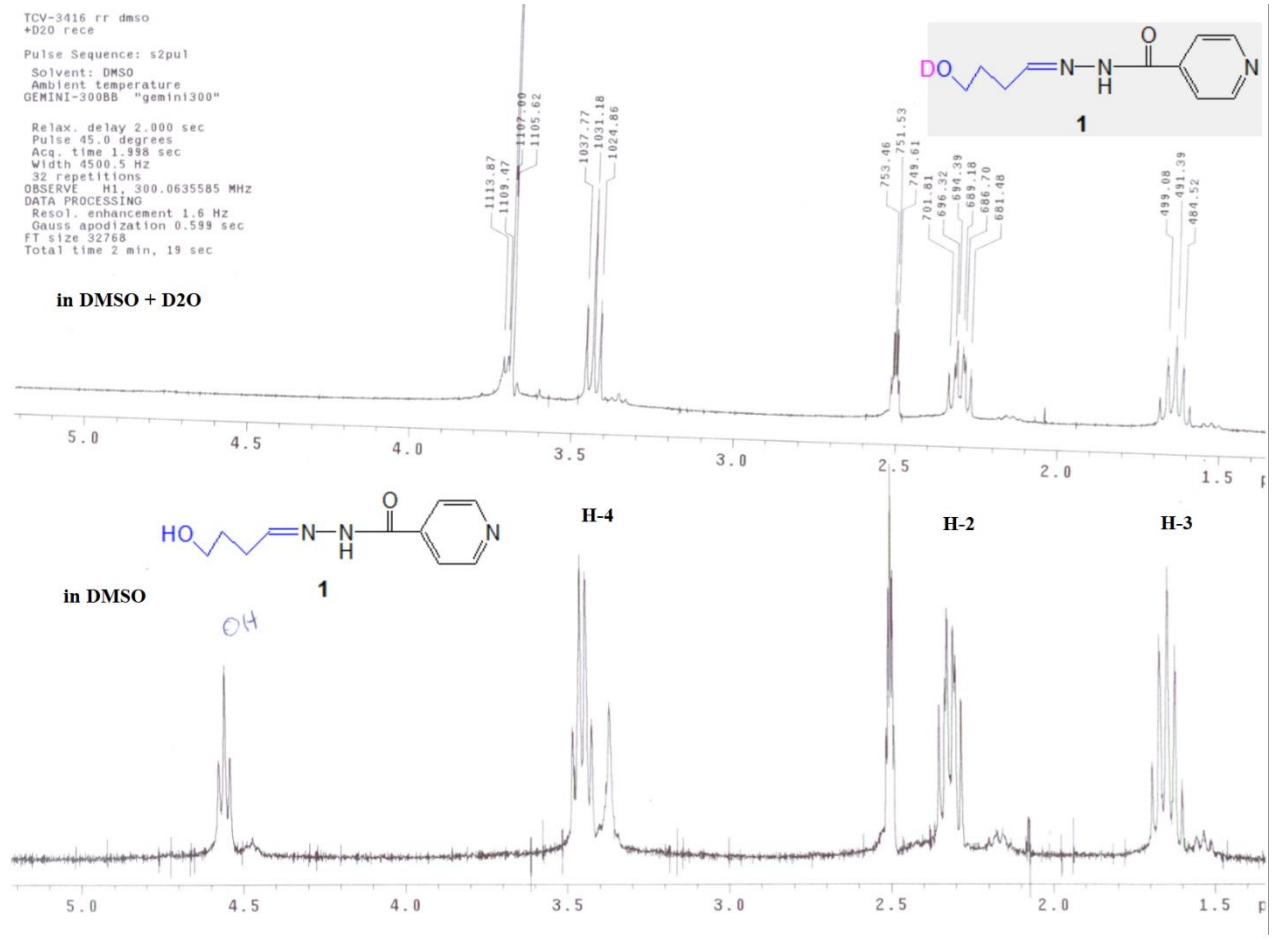


1.8. ^{1}H, ^{13}C, COSY and HETCOR-NMR spectra in DMSO of *crystallized compound* **1** *directly from the crude product* (without LPC) of the reaction of INH with THF[X] reduced with triphenylphosphine

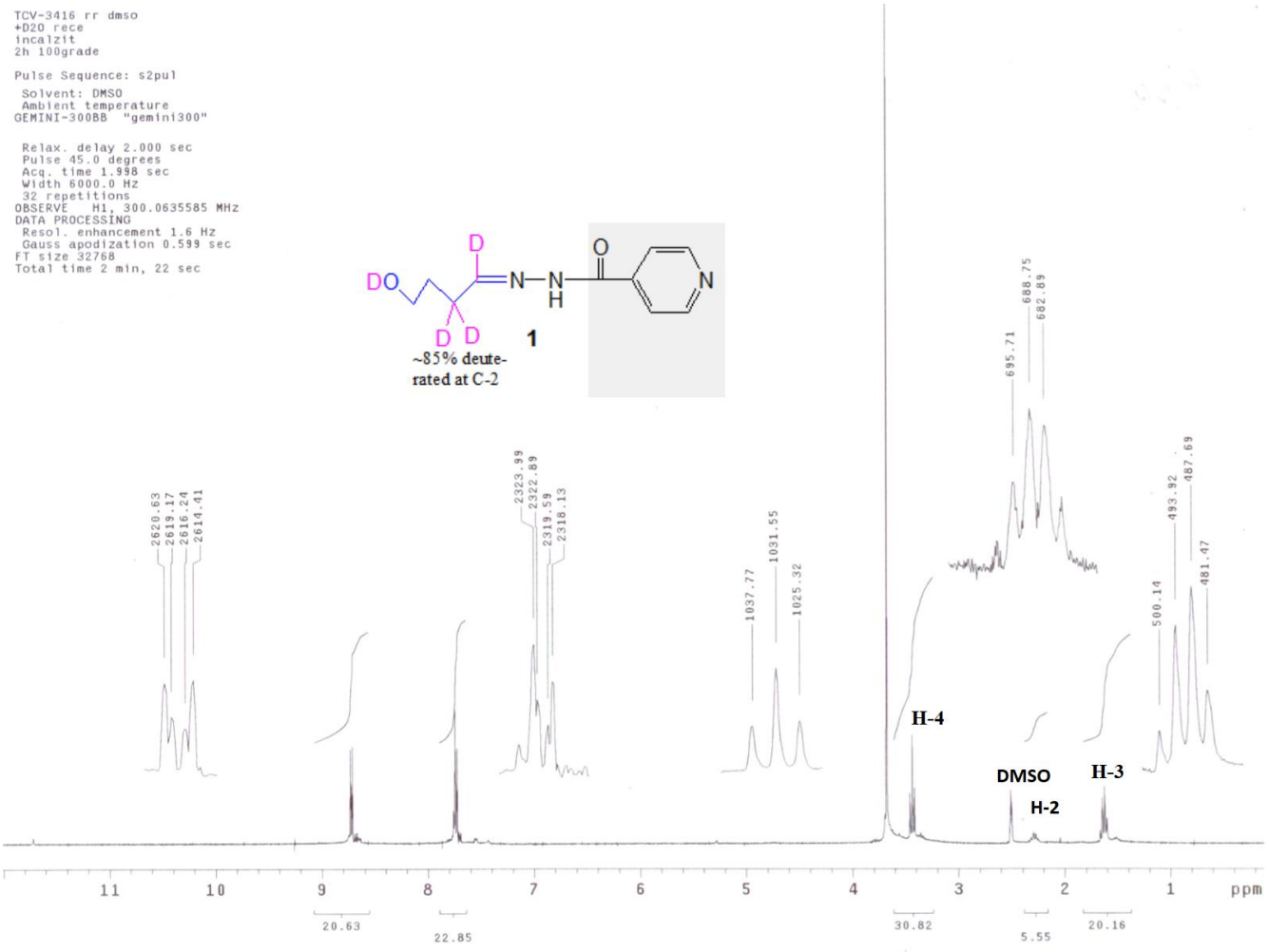
In DMSO + D_2O at r. t.

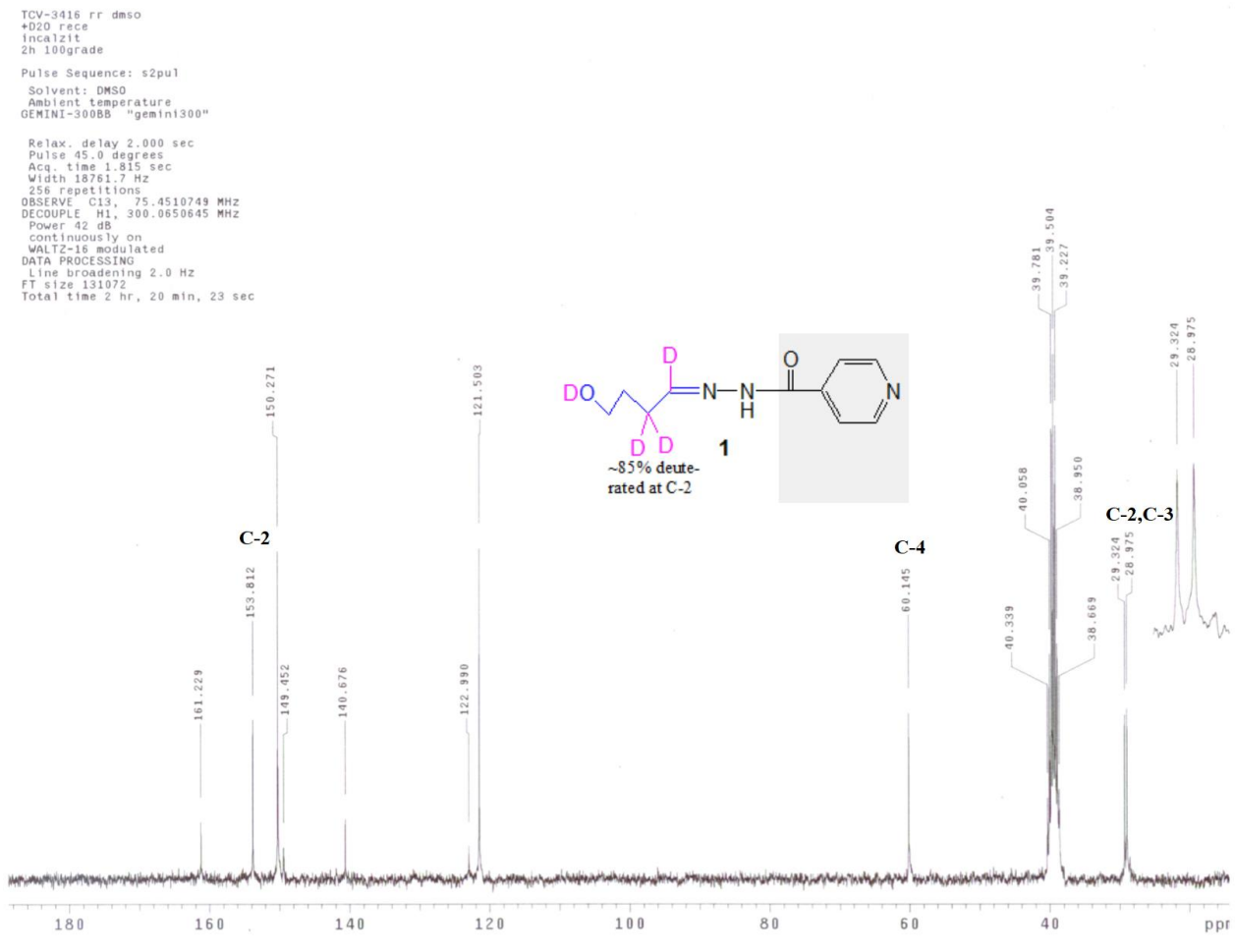




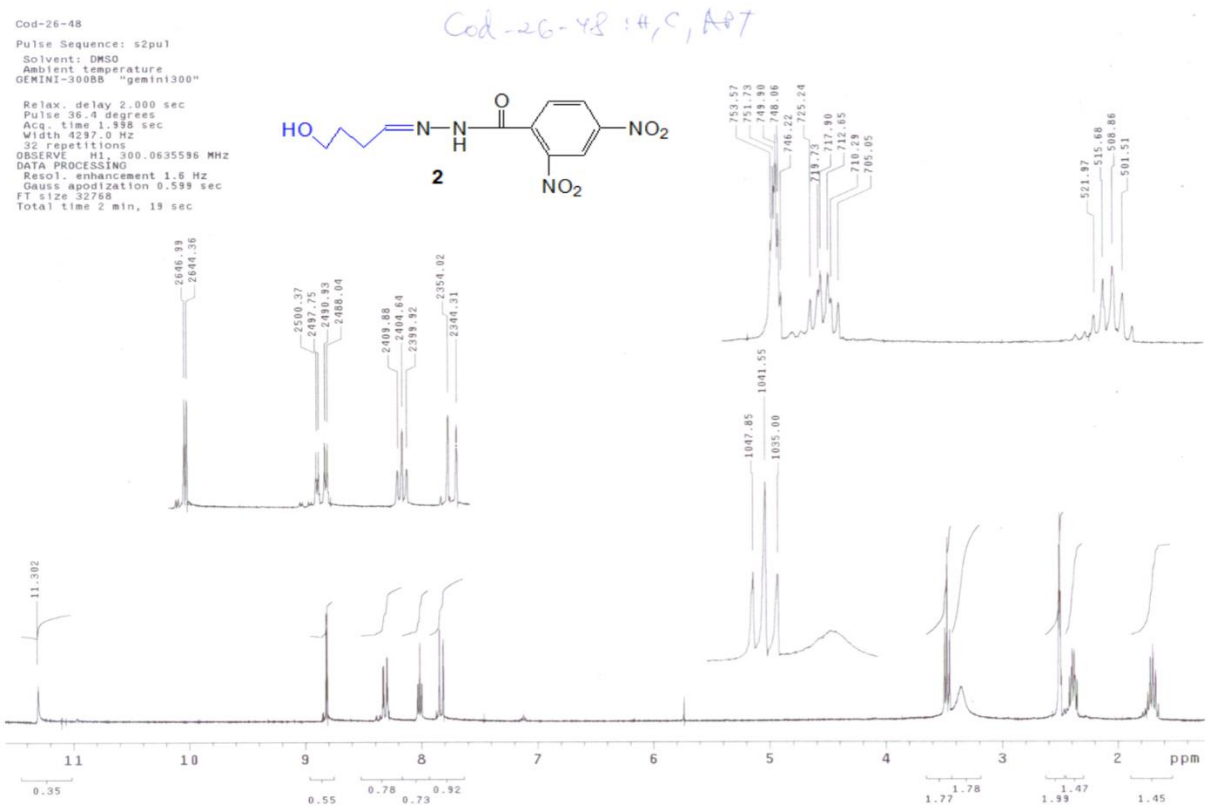


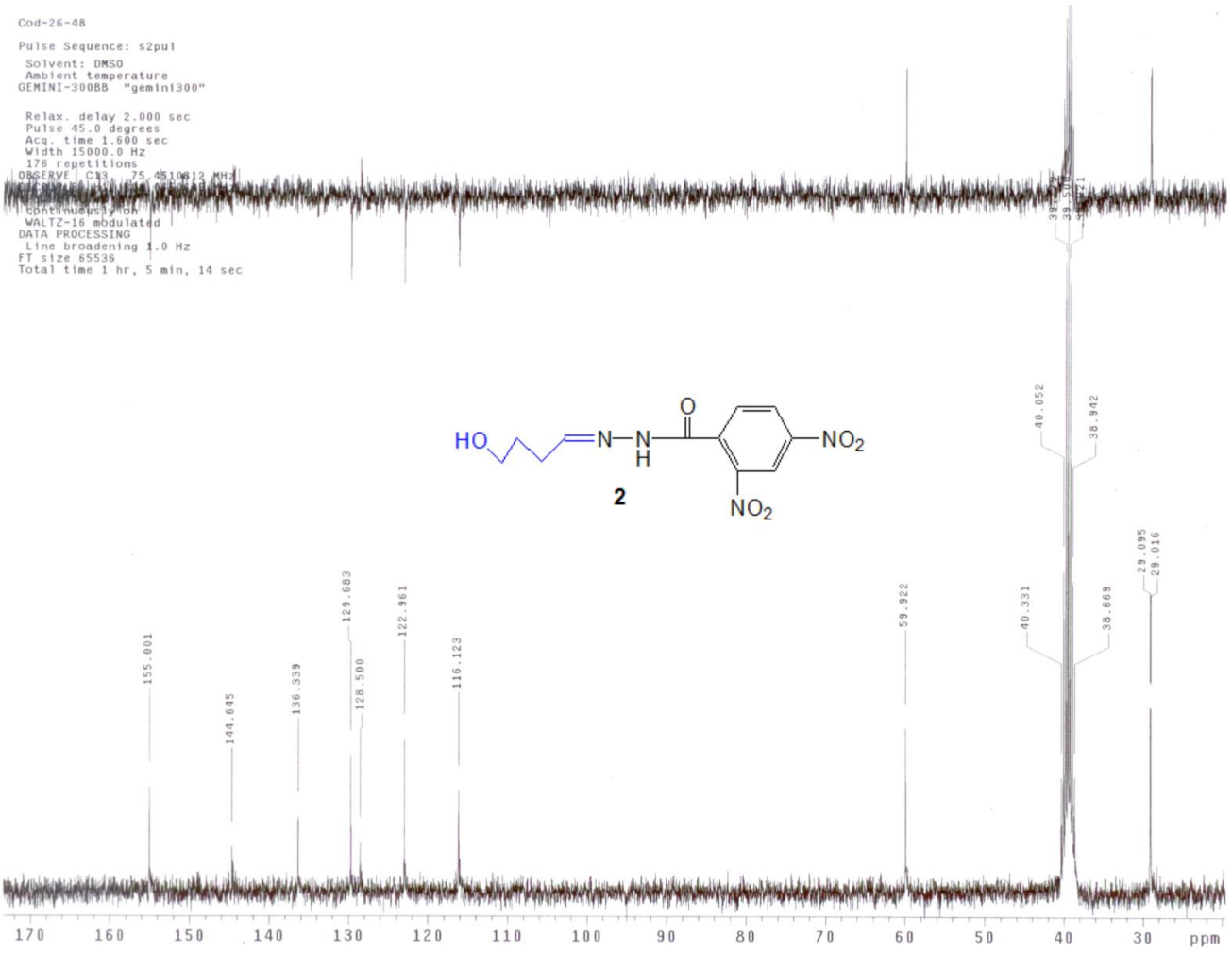
16 h r.t., then 2 h at 100˚C:

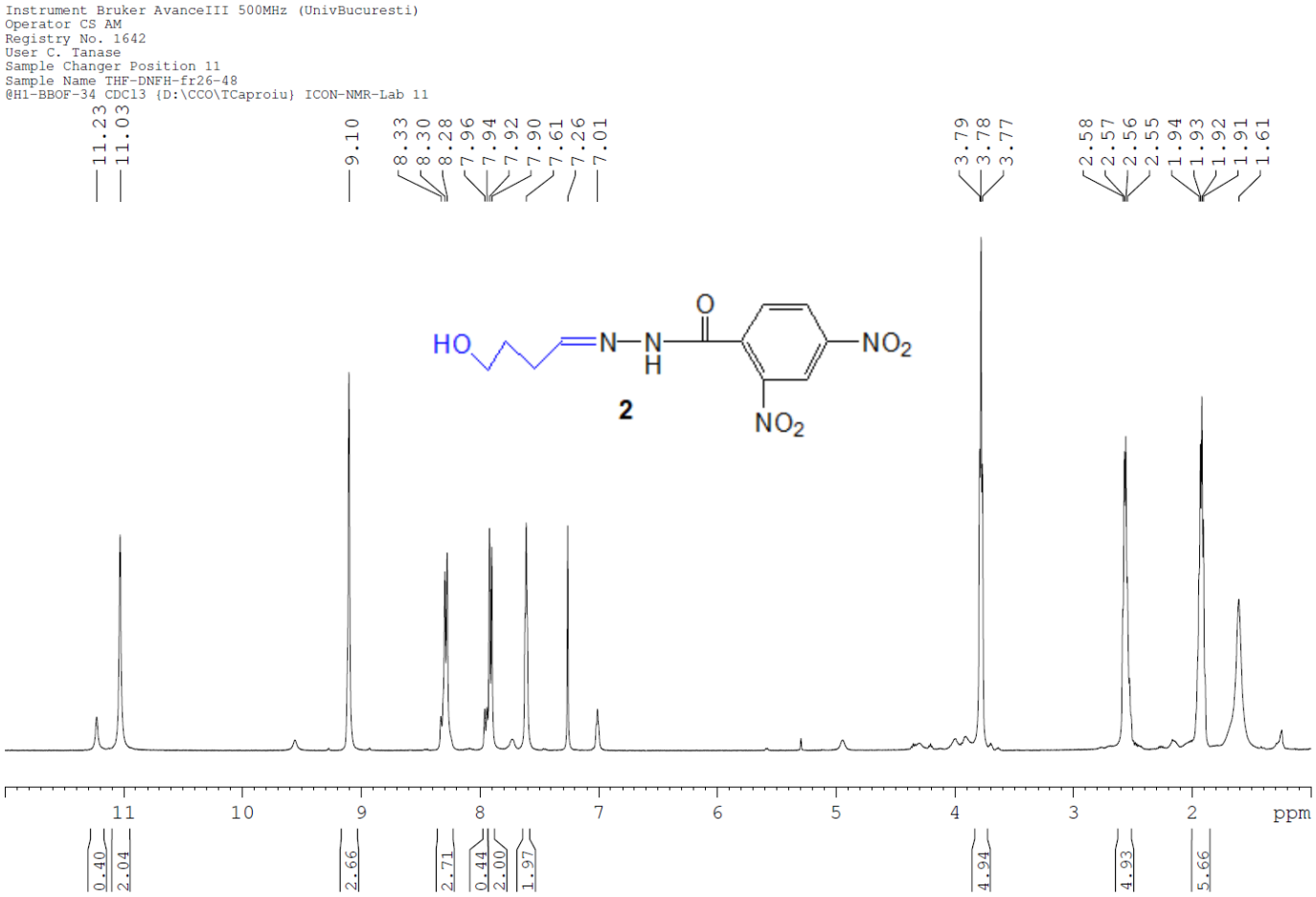

TCV-3416 rr dmso
+D2O rece
incalzit
2h 100grade
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
GEMINI-300BB "gemini300"
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 6000.0 Hz
32 repetitions
OBSERVE H1, 300.0635585 MHz
DATA PROCESSING
Resol. enhancement 1.6 Hz
Gauss apodization 0.599 sec
FT size 32768
Total time 2 min, 22 sec
DO
D
N
O
H
1
~85% deute-
rated at C-2
2620.63
2619.17
2616.24
2614.41
2323.99
2322.89
2319.59
2318.13
1037.77
1031.55
1025.32
695.71
688.75
682.89
500.14
493.92
487.69
481.47
H-4
DMSO
H-2
H-3
11
10
9
8
7
6
5
4
3
2
1
ppm
20.63
22.85
30.82
5.55
20.16

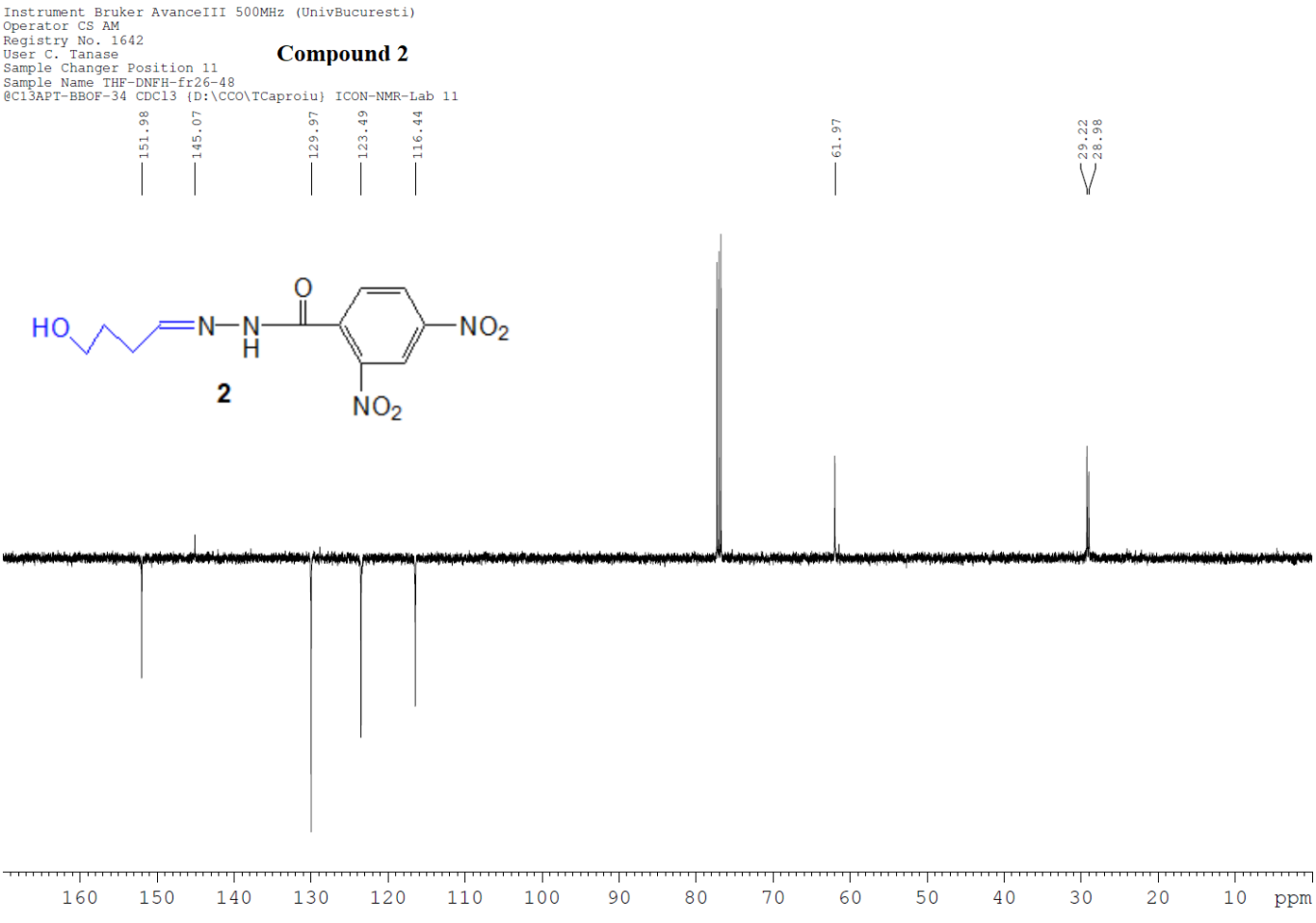

TCV-3416 rr dmso
+D2O rece
incalzit
2h 100grade
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
GEMINI-300BB "gemini300"
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
256 repetitions
OBSERVE C13, 75.4510749 MHz
DECOUPLE H1, 300.0650645 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 20 min, 23 sec
DO
D
N
O
H
1
~85% deute-
rated at C-2
150.271
121.503
153.812
149.452
140.676
122.980
161.229
C-2
C-4
C-2,C-3
60.145
40.339
40.058
39.781
39.504
39.227
38.950
38.669
29.324
28.975
180
160
140
120
100
80
60
40
ppm

1.9. ^{1}H- and ^{13}C-NMR spectra in DMSO and $CDCl_3$ of the crystallized compound **2** obtained by reaction of 2,4-DNPH with THF[X]



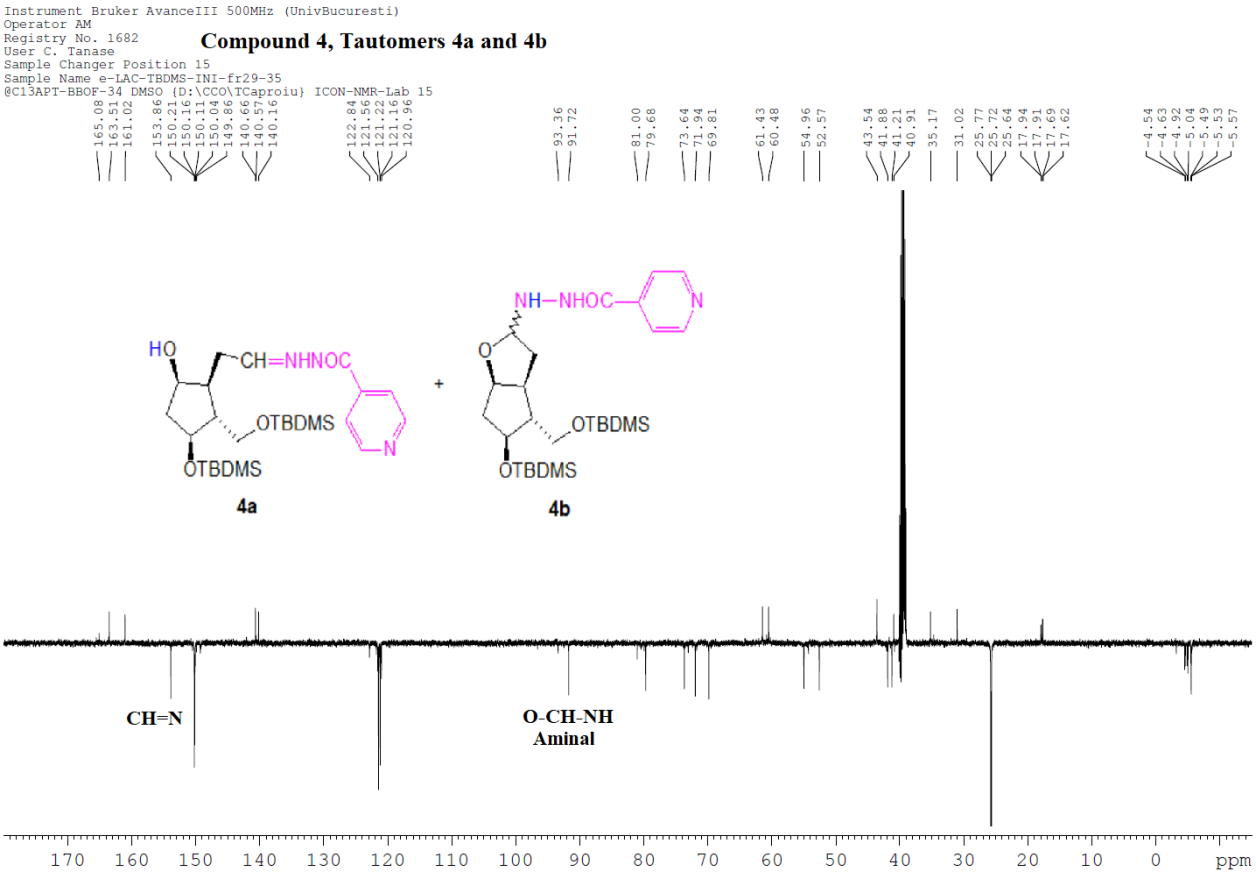


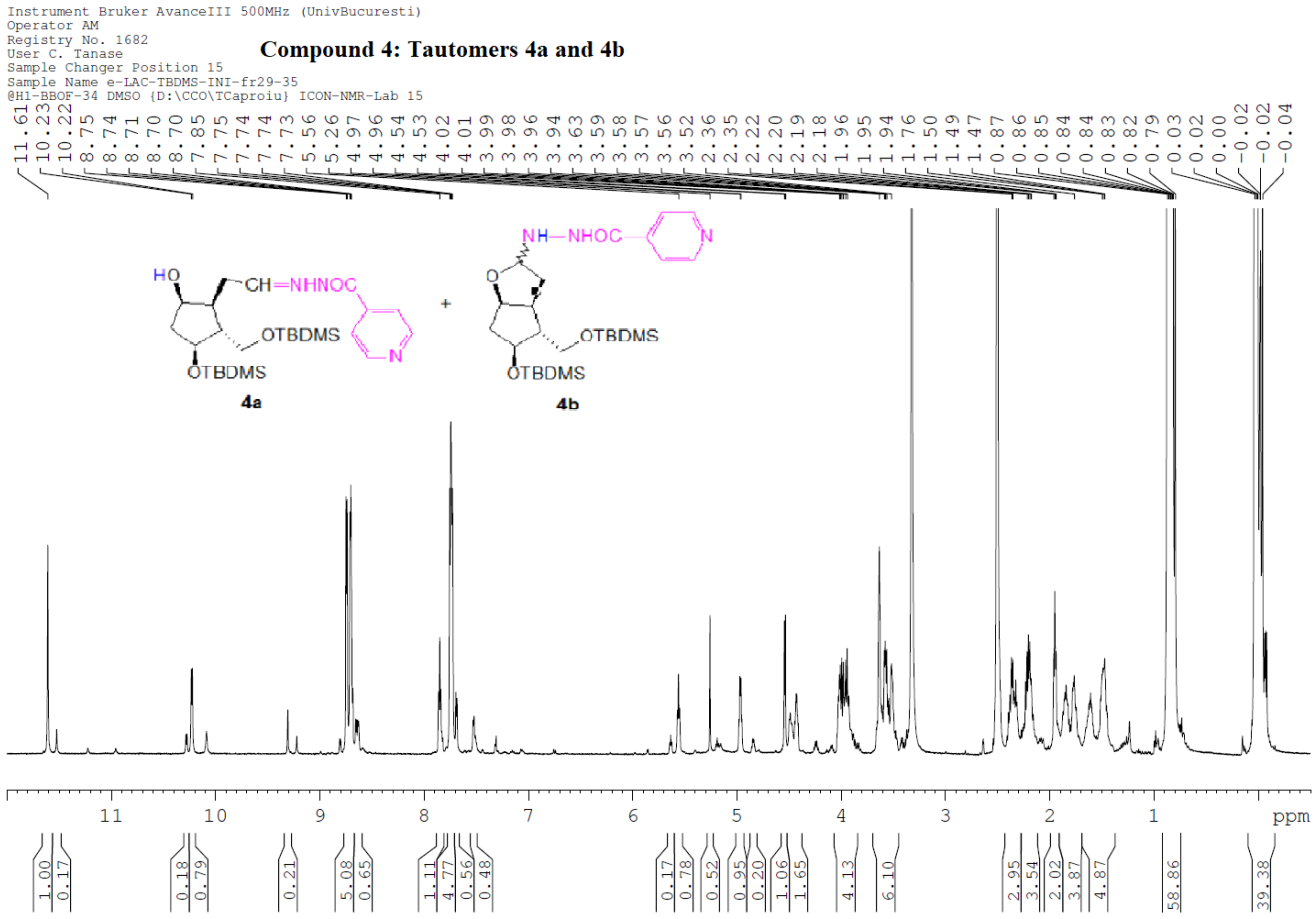




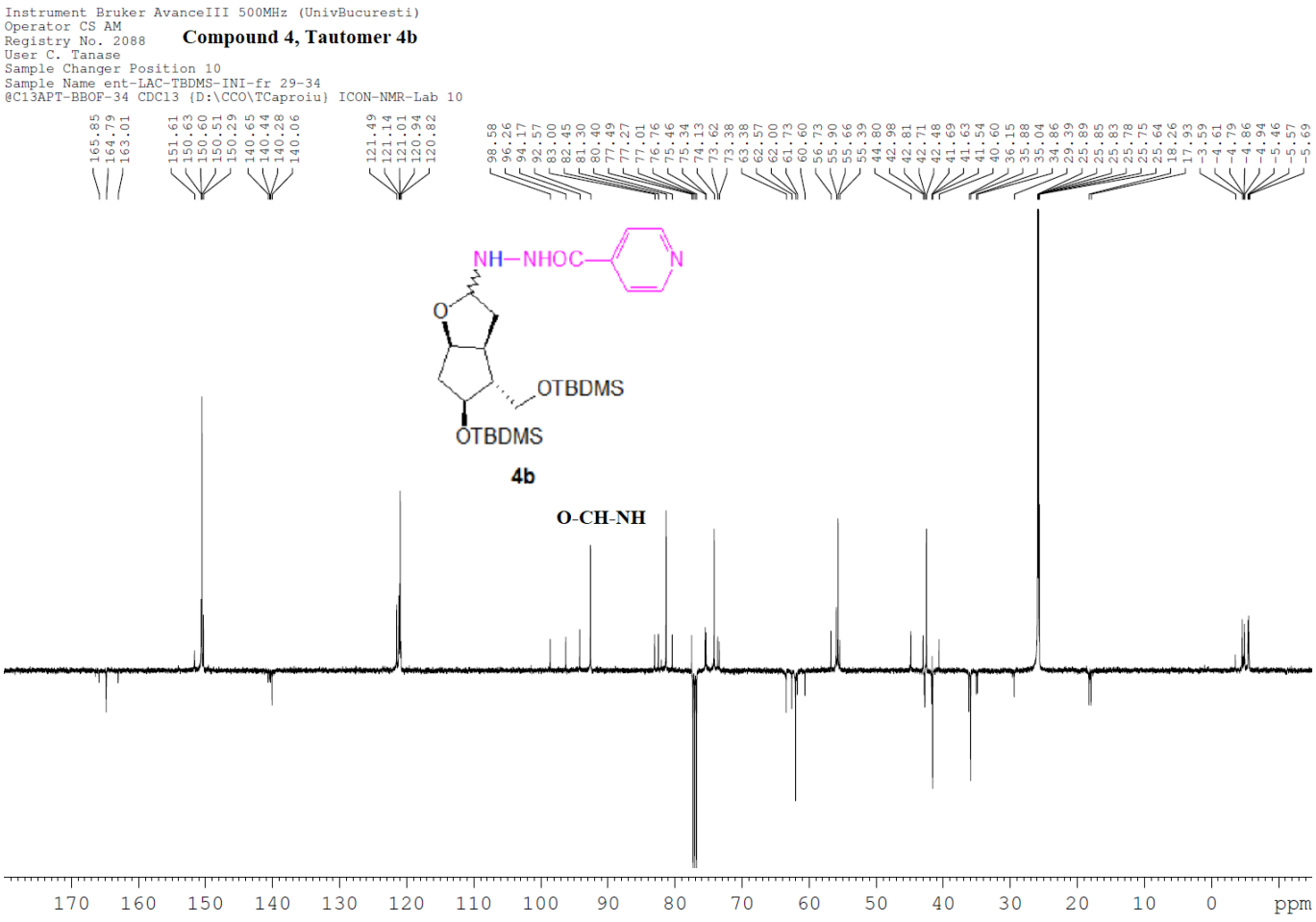
1.10. ^{1}H- and ^{13}C-NMR spectra in DMSO and $CDCl_3$ of the compound **4**, obtained by reaction of lactol **3** with INH.

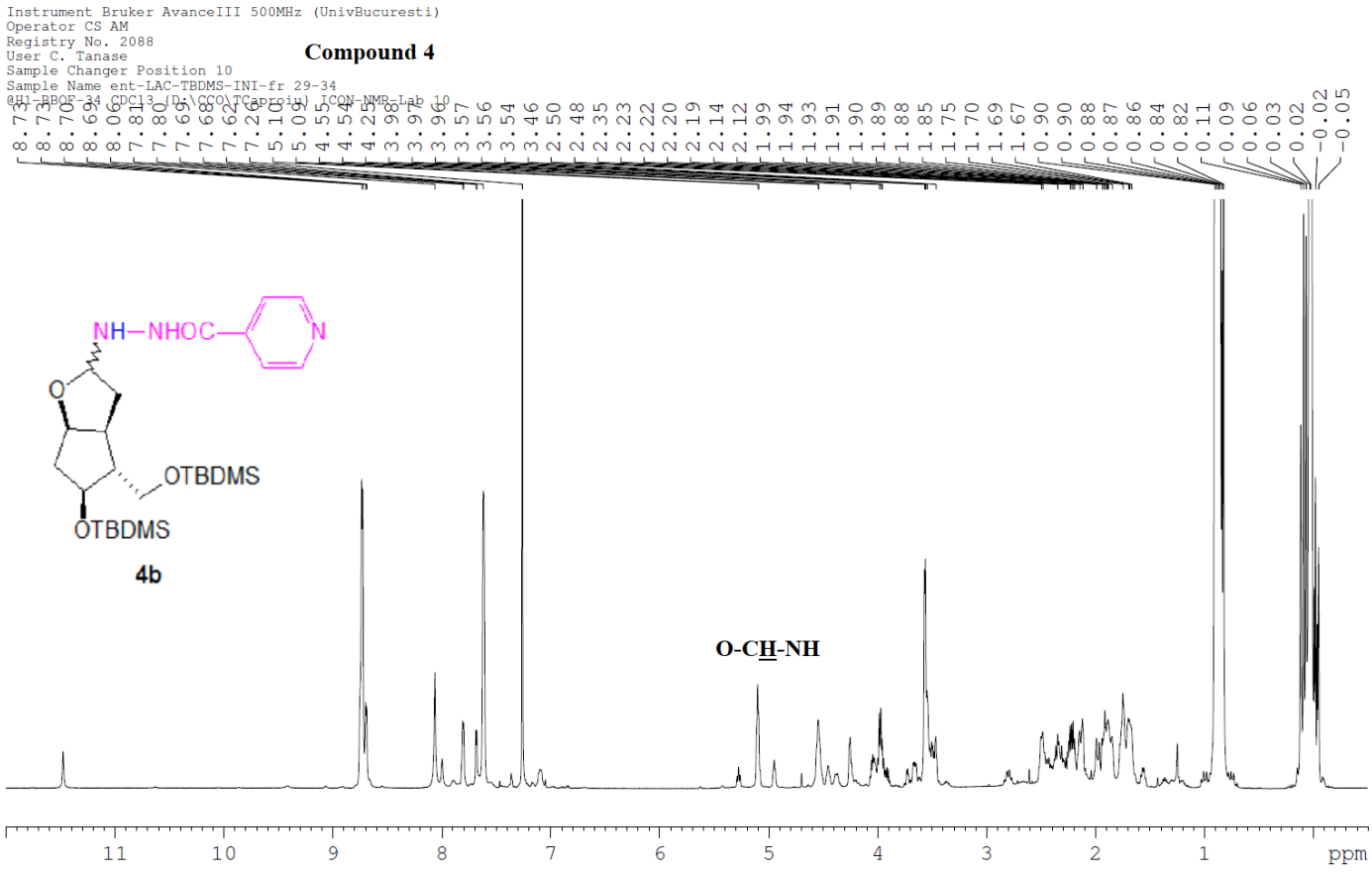
-in DMSO:





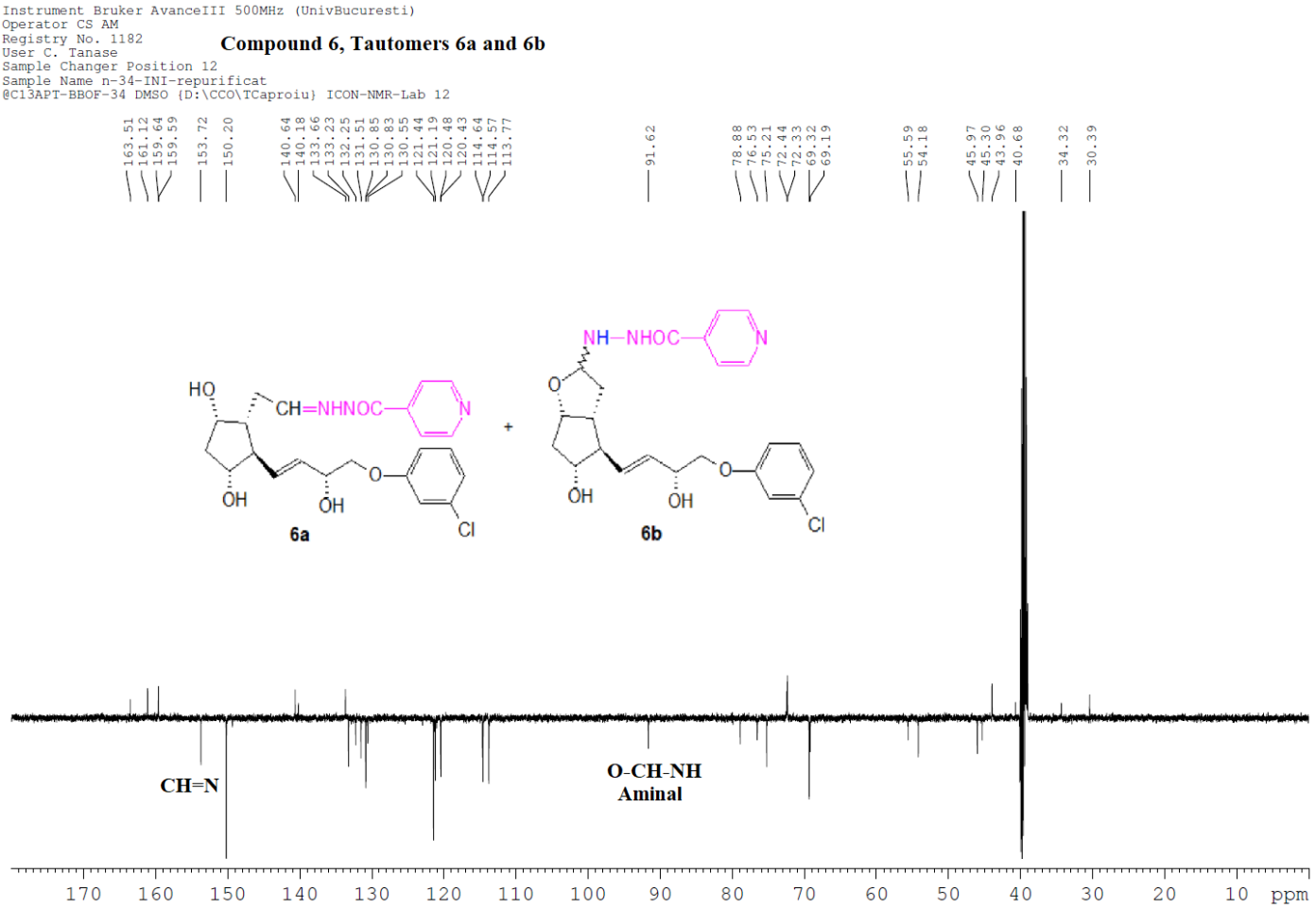
-in $CDCl_3$:

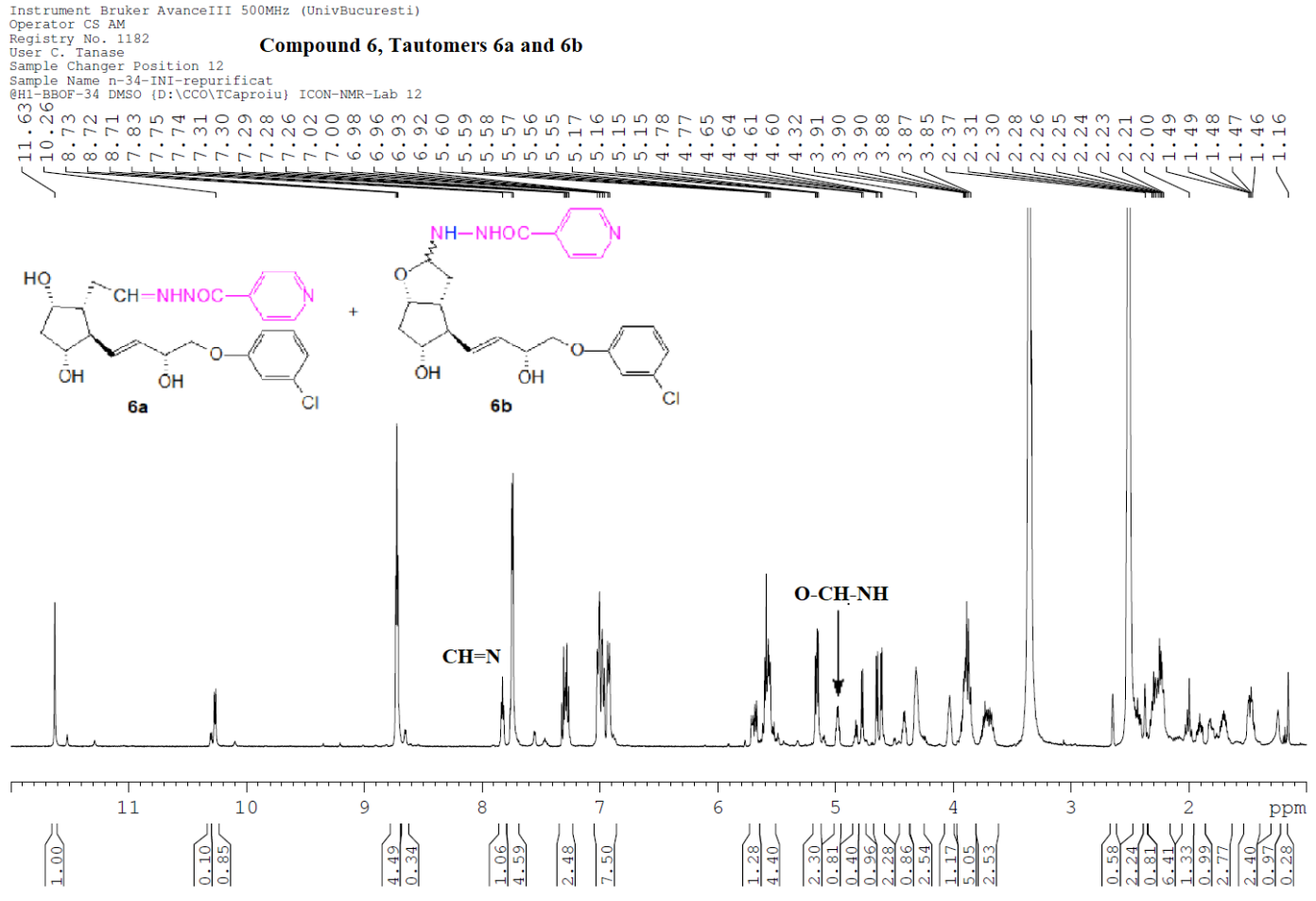




1.11. ^{1}H- and ^{13}C-NMR spectra in DMSO and $CDCl_3$ of the compound **6**, obtained by reaction of lactol **5** with INH.

-in DMSO:

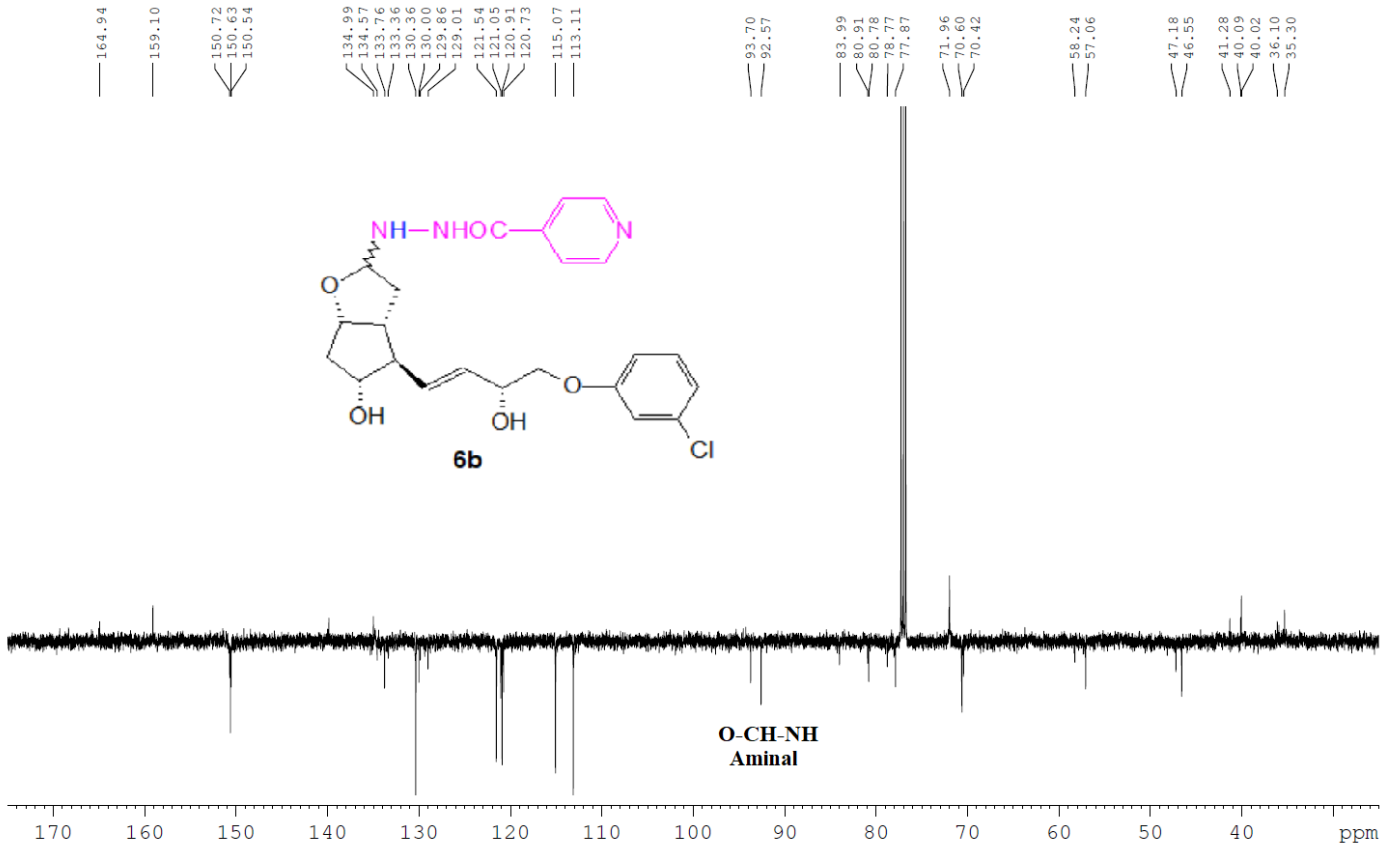

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1182
User C. Tanase
Sample Changer Position 12
Sample Name n-34-INI-repurificat
@C13APT-BBOF-34 DMSO {D:\CCO\TCaproiu} ICON-NMR-Lab 12
Compound 6, Tautomers 6a and 6b
163.51
161.12
159.64
159.59
153.72
150.20
140.64
140.18
133.66
133.23
132.25
131.51
130.85
130.83
130.55
121.44
121.19
120.48
120.43
114.64
114.57
113.77
91.62
78.88
76.53
75.21
72.44
72.33
69.32
69.19
55.59
54.18
45.97
45.30
43.96
40.68
34.32
30.39
HO
CH=NHNOC
N
O
OH
OH
Cl
6a
+
NH—NHOC
6b
CH=N
O-CH-NH
Aminal
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1182
User C. Tanase
Sample Changer Position 12
Sample Name n-34-INI-repurificat
@H1-BBOF-34 DMSO {D:\CCO\TCaproiu} ICON-NMR-Lab 12
Compound 6, Tautomers 6a and 6b
11.63
10.26
8.73
8.72
8.71
7.83
7.75
7.74
7.31
7.30
7.29
7.28
7.26
7.02
7.00
6.98
6.96
6.93
6.92
5.60
5.59
5.58
5.57
5.56
5.55
5.17
5.16
5.15
5.15
4.78
4.77
4.65
4.64
4.61
4.60
4.32
3.91
3.90
3.90
3.88
3.87
3.85
2.37
2.31
2.30
2.28
2.26
2.25
2.24
2.23
2.21
2.00
1.49
1.49
1.48
1.47
1.46
1.16
HO
CH=NHNOC
N
O
OH
OH
Cl
6a
+
NH—NHOC
6b
CH=N
O-CH-NH
11
10
9
8
7
6
5
4
3
2
ppm
1.00
0.10
0.85
4.49
0.34
1.06
4.59
2.48
7.50
1.28
4.40
2.30
0.81
0.40
0.96
2.28
0.86
2.54
1.17
5.05
2.53
0.58
2.24
0.81
6.41
1.33
0.99
2.77
2.40
0.97
0.28

-in $CDCl_3$:

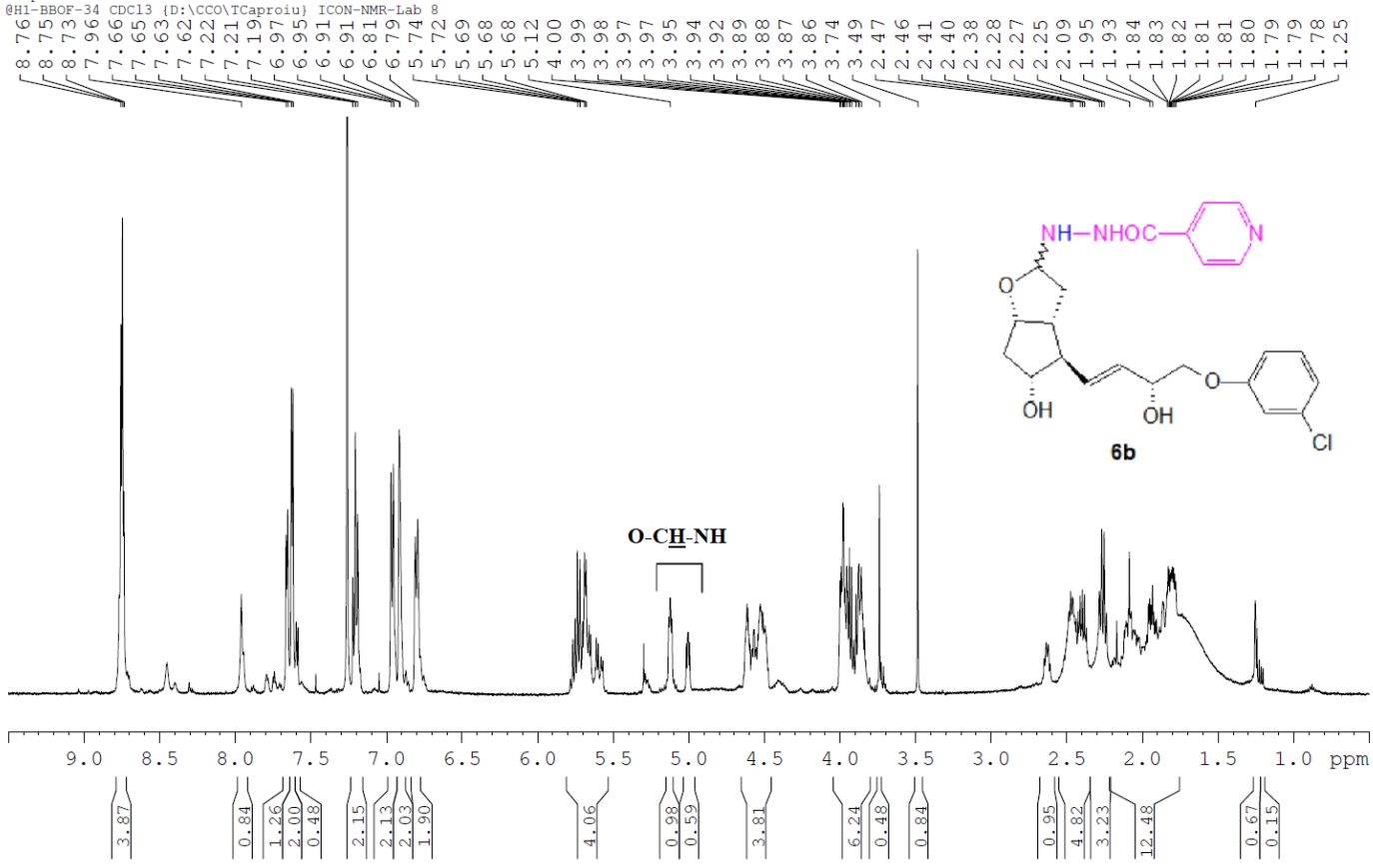
Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1644
User C. Tanase
Sample Changer Position 8
Sample Name RAC-34-INI-CDCl3
@C13APT-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 8

Compound 6, Tautomer 6b



Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS AM
Registry No. 1644
User C. Tanase
Sample Changer Position 8
Sample Name RAC-34-INI-CDCl3
@H1-BBOF-34 CDCl3 {D:\CCO\TCaproiu} ICON-NMR-Lab 8

Compound 6, Tautomer 6b



2. X-Ray crystallography of the compound: Figure 5S, Table 1S, Table 2S, Table 1-8

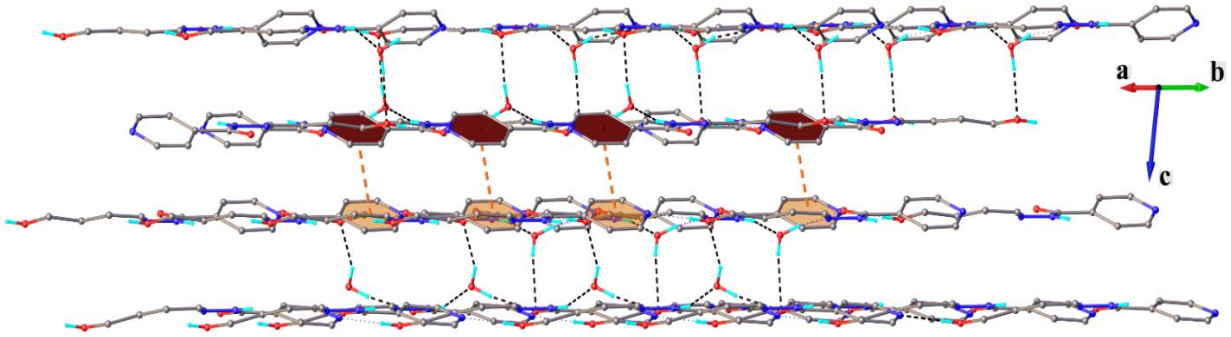


Figure 5S. Partial view of crystal packing showing the π-π stacking between 2D layers. Centroid-to-centroid distances are shown as dashed orange lines. The aromatic rings of **C** and **B** molecules are in brown and orange, respectively.

Table 1S. Bond distances (Å) and angles (°).

Molecule	**A**	**B**	**C**	**D**
O1-C6	1.234(3)	1.230(3)	1.221(3)	1.224(3)
O2-C10	1.410(3)	1.416(3)	1.434(3)	1.424(3)
N1-C1	1.327(3)	1.341(3)	1.336(3)	1.328(4)
N1-C5	1.344(3)	1.343(3)	1.323(3)	1.345(3)
N2-N3	1.394(3)	1.390(3)	1.396(3)	1.396(3)
N2-C6	1.334(3)	1.329(3)	1.352(3)	1.338(3)
N3-C7	1.273(3)	1.268(3)	1.273(3)	1.276(3)
C1-C2	1.389(3)	1.385(4)	1.368(4)	1.380(3)
C2-C3	1.384(3)	1.387(4)	1.389(4)	1.386(3)
C3-C4	1.386(4)	1.377(3)	1.391(3)	1.382(4)
C3-C6	1.504(3)	1.518(3)	1.502(4)	1.504(3)
C4-C5	1.374(3)	1.372(4)	1.379(4)	1.383(4)
C7-C8	1.483(3)	1.483(3)	1.492(3)	1.478(3)
C8-C9	1.527(3)	1.532(3)	1.517(3)	1.518(3)
C9-C10	1.513(3)	1.521(3)	1.506(3)	1.504(3)
C1-N1-C5	116.6(2)	116.0(2)	116.8(2)	117.1(2)
C6-N2-N3	**118.2(2)**	**118.6(2)**	**117.2(2)**	**118.4(2)**
C7-N3-N2	**115.4(2)**	**115.4(2)**	**115.0(2)**	**114.8(2)**
N1-C1-C2	123.7(2)	124.1(2)	123.3(3)	123.8(2)
C3-C2-C1	119.0(2)	118.4(3)	119.9(2)	118.8(3)
C2-C3-C4	117.7(2)	123.6(2)	116.9(2)	123.9(2)
C2-C3-C6	124.2(2)	118.2(2)	117.7(2)	118.2(2)
C4-C3-C6	118.1(2)	118.2(2)	125.4(2)	117.9(2)
C5-C4-C3	119.2(2)	119.5(2)	118.9(3)	119.0(2)
N1-C5-C4	123.8(2)	123.8(3)	124.1(2)	123.0(3)
O1-C6-N2	**123.9(2)**	**123.7(2)**	**123.1(2)**	**124.8(2)**
O1-C6-C3	**119.3(2)**	**119.2(2)**	**120.3(2)**	**119.8(2)**
N2-C6-C3	**116.8(2)**	**117.1(2)**	**116.6(2)**	**115.4(2)**
N3-C7-C8	**120.4(2)**	**121.6(2)**	**120.8(2)**	**120.2(2)**
C7-C8-C9	115.3(2)	114.4(2)	115.3(2)	115.7(2)
C10-C9-C8	112.1(2)	112.4(2)	112.5(2)	111.1(2)
O2-C10-C9	108.5(2)	107.9(2)	107.8(2)	109.5(2)

Table 2S. H-bonds parameters.

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*	Symmetry code
O2A-H···N1A[1]	0.82	2.07	2.882(3)	174.0	*x*, *y*, *z*
N2A-H···O4*w*	0.86	1.99	2.809(3)	159.7	*x*, *y*, *z*
O2C-H···N1C[2]	0.82	2.00	2.816(3)	176.5	*x*, *y*, *z*
N2C-H···O1*w*	0.86	2.00	2.833(3)	162.9	*x*, *y*, *z*
O2B-H···N1B[1]	0.82	1.97	2.792(3)	179.0	*x*, *y*, *z*
N2B-H···O3*w*[3]	0.86	2.04	2.869(3)	162.8	*x*, *y*, *z*
O2D-H···N1D[1]	0.85	1.98	2.791(2)	158.7	*x*, *y*, *z*
N2D-H···O2*w*	0.86	2.03	2.821(2)	152.5	*x*, *y*, *z*
O1*w*-H···O2D[3]	0.85	2.00	2.838(3)	170.1	*x*, *y*, *z*
O1*w*-H···O1C[4]	0.85	2.16	2.873(2)	141.8	*x*, *y*, *z*
O1*w*-H···N3C[4]	0.85	2.54	3.275(3)	144.5	*x*, *y*, *z*
O3*w*-H···O1A	0.85	2.45	3.293(3)	171.3	*x*, *y*, *z*
O3*w*-H···O1B	0.85	1.99	2.814(3)	163.9	*x*, *y*, *z*
O3*w*-H···N3B	0.85	2.69	3.256(3)	125.6	*x*, *y*, *z*
O2w-H···O1D[3]	0.85	2.03	2.850(2)	161.4	*x*, *y*, *z*
O2*w*-H···O2C[4]	0.85	1.97	2.819(3)	174.1	*x*, *y*, *z*
O4*w*-H···O1A[3]	0.85	2.00	2.831(2)	167.3	*x*, *y*, *z*
O4*w*-H···O2B[3]	0.86	1.97	2.768(3)	153.5	*x*, *y*, *z*

Symmetry codes: [1]1 + *x*, -1 + *y*, + *z*; [2]-1 + *x*, 1 + *y*, + *z*; [3]-1 + *x*, + *y*, + *z*; [4]1 + *x*, + *y*, + *z*.

* *Crystal data for* ***1***: $C_{40}H_{60}N_{12}O_{12}$, *Mr* = 901.00 g mol^{-1}, size 0.40×0.20×0.20 mm^3, triclinic, space group *P*1, *a* = 6.6116(2) Å, *b* = 12.1182(5) Å, *c* = 15.0179(7) Å, α= 110.945(4)°β= 98.955(3)°, γ= 92.334(3)°, *V* = 1103.98(7) Å^3, *Z* = 1, ρ_{calcd} = 1.355 g cm^{-3}, μ(Mo*K*α) = 0.102 mm^{-1}, *F*(000) = 480, 16607 reflections in *h*(-7/7), *k*(-14/14), *l*(-17/17), measured in the range 2.96 ≤ 2Θ ≤ 50.04, T = 293 K, completeness Θ_{max}=99.99%, 7727 independent reflections, R_{int} = 0.0272, 577 parameters, 3 restraints, R_{1obs}=0.0455, wR_{2obs} = 0.0831, R_{1all} = 0.0533, wR_{2all} = 0.0978, GoF = 1.029, largest difference peak and hole: 0.18/-0.19 e A^{-3}.

shI_3363_CoTa for Compound 1.

Table 1 Crystal data and structure refinement for shI_3363_CoTa.

Identification code	shI_3363_CoTa
Empirical formula	$C_{40}H_{60}N_{12}O_{12}$
Formula weight	901.00
Temperature/K	200.00(10)
Crystal system	triclinic
Space group	P1
a/Å	6.6116(2)
b/Å	12.1182(5)
c/Å	15.0179(7)
α/°	110.945(4)
β/°	98.955(3)
γ/°	92.334(3)
Volume/Å^3	1103.98(7)
Z	1
ρ_{calc}g/cm^3	1.355
μ/mm^{-1}	0.102
F(000)	480.0

Crystal size/mm^3	0.4 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.96 to 50.04
Index ranges	-7 ≤ h ≤ 7, -14 ≤ k ≤ 14, -17 ≤ l ≤ 17
Reflections collected	16607
Independent reflections	7727 [R_{int} = 0.0272, R_{sigma} = 0.0480]
Data/restraints/parameters	7727/3/577
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0455, wR_2 = 0.0931
Final R indexes [all data]	R_1 = 0.0533, wR_2 = 0.0978
Largest diff. peak/hole / e Å^{-3}	0.18/-0.19
Flack parameter	0.2(8)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for shI_3363_CoTa. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1A	11559(2)	12206.0(16)	13737.7(15)	35.4(5)
O2A	15057(3)	7443.8(17)	14100.5(16)	45.5(6)
N1A	6468(3)	15156.8(19)	13878.1(16)	27.7(5)
N2A	8636(3)	11103.2(18)	13657.2(15)	19.9(5)
N3A	9728(3)	10146.8(19)	13668.9(15)	22.0(5)
C1A	5625(4)	14272(2)	14067.2(19)	25.2(6)
C2A	6548(4)	13244(2)	14005.4(19)	24.0(6)
C3A	8473(4)	13130(2)	13749.5(17)	18.6(5)
C4A	9370(4)	14051(2)	13552.3(18)	24.9(6)
C5A	8331(4)	15029(2)	13623.1(19)	27.9(6)
C6A	9684(4)	12095(2)	13709.9(18)	21.6(6)
C7A	8641(4)	9215(2)	13592.4(19)	24.1(6)
C8A	9633(4)	8148(2)	13619(2)	24.6(6)
C9A	11981(4)	8277(2)	13762(2)	28.2(6)
C10A	12900(4)	7271(2)	14001(2)	29.3(6)
O1C	-380(3)	5235.4(18)	8940.7(16)	37.6(5)
O2C	-3817(2)	10045.6(16)	8676.9(14)	32.7(5)
N1C	4517(3)	2197(2)	8843.6(17)	28.7(6)
N2C	2444(3)	6150.2(18)	8717.7(16)	22.2(5)
N3C	1370(3)	7120.1(19)	8721.7(16)	22.6(5)
C1C	2825(4)	2468(2)	9227(2)	31.9(7)
C2C	1826(4)	3435(2)	9226.2(19)	26.7(6)
C3C	2590(4)	4205(2)	8831.0(19)	22.7(6)
C4C	4356(4)	3928(2)	8435(2)	29.1(7)
C5C	5244(4)	2928(3)	8464(2)	33.1(7)
C6C	1414(4)	5241(2)	8836.7(19)	24.2(6)
C7C	2454(4)	8003(2)	8706(2)	23.8(6)
C8C	1511(4)	9103(2)	8712(2)	26.2(6)
C9C	-804(3)	9039(2)	8654.2(19)	20.3(6)
C10C	-1621(4)	10219(2)	8786(2)	24.5(6)
O1B	9433(3)	13581.8(17)	11076.9(15)	37.8(5)
O2B	12740(2)	8703.7(15)	11327.0(13)	28.3(4)
N1B	4409(3)	16565(2)	11118.1(17)	29.8(6)

N2B	6607(3)	12647.1(18)	11271.9(15)	22.9(5)
N3B	7641(3)	11669.9(19)	11267.8(15)	21.5(5)
C1B	3699(4)	15817(2)	11502(2)	31.9(7)
C2B	4633(4)	14829(2)	11540(2)	27.8(6)
C3B	6430(4)	14598(2)	11169.2(19)	22.3(6)
C4B	7195(4)	15367(2)	10784(2)	26.3(6)
C5B	6149(4)	16314(2)	10763(2)	30.0(6)
C6B	7624(4)	13558(2)	11181.5(19)	24.8(6)
C7B	6507(4)	10741(2)	11150.8(19)	23.0(6)
C8B	7386(4)	9618(2)	11101(2)	25.0(6)
C9B	9742(4)	9707(2)	11255.2(19)	21.6(6)
C10B	10562(4)	8518(2)	11137.0(19)	21.7(6)
O1D	11707(2)	9785.4(16)	6165.1(15)	36.4(5)
O2D	15057(2)	4800.4(15)	6312.2(13)	32.0(5)
N1D	6430(3)	12592(2)	6114.2(17)	31.5(6)
N2D	8806(3)	8688.8(18)	6127.6(15)	22.4(5)
N3D	9885(3)	7723.5(19)	6130.0(15)	22.2(5)
C1D	5522(4)	11486(3)	5729(2)	32.3(7)
C2D	6511(4)	10505(2)	5730(2)	30.3(6)
C3D	8585(4)	10667(2)	6134.9(18)	21.5(6)
C4D	9565(4)	11811(2)	6524(2)	31.6(6)
C5D	8440(4)	12744(2)	6510(2)	35.5(7)
C6D	9853(4)	9668(2)	6146.3(18)	22.0(6)
C7D	8807(4)	6848(2)	6167.1(18)	22.8(6)
C8D	9783(4)	5789(2)	6213(2)	23.5(6)
C9D	12056(4)	5803(2)	6156(2)	25.4(6)
C10D	12868(4)	4669(2)	6178(2)	26.5(6)
O1W	6384(3)	6404.3(16)	8252.5(15)	37.9(5)
O3W	12590(3)	12407.3(17)	11722.3(16)	45.4(6)
O2W	4976(2)	8560.8(17)	6710.6(14)	35.1(5)
O4W	4358(2)	10522.6(17)	13069.6(15)	42.4(5)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for shI_3363_CoTa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1A	16.1(9)	24.2(10)	68.0(14)	17.6(10)	11.0(9)	5.8(7)
O2A	25.9(10)	30.7(11)	84.3(17)	25.8(11)	9.7(10)	10.3(8)
N1A	26.0(11)	23.3(13)	31.8(14)	9.3(11)	1(1)	6.7(9)
N2A	13.4(10)	17.8(12)	30.9(13)	10.1(10)	7.5(9)	6.3(8)
N3A	20.7(11)	19.2(12)	29.2(13)	11.5(10)	5.8(9)	6.9(9)
C1A	17.5(12)	22.5(15)	34.0(16)	8.1(13)	4.4(11)	5.7(10)
C2A	20.4(13)	23.8(15)	30.6(15)	12.8(13)	5.8(11)	1.4(11)
C3A	20.8(13)	15.2(13)	15.6(13)	1.6(11)	0.7(10)	1(1)
C4A	21.0(12)	24.0(15)	30.4(15)	9.1(12)	8.2(11)	5.9(11)
C5A	30.1(14)	20.8(15)	35.1(16)	14.0(13)	4.1(12)	0.3(11)
C6A	20.5(13)	19.5(14)	25.4(15)	7.0(12)	8.6(11)	4.3(11)
C7A	20.7(13)	22.8(16)	30.7(15)	10.8(13)	6.8(11)	6.7(11)
C8A	28.1(14)	18.7(14)	28.6(15)	10.1(12)	6.8(12)	2.6(11)

C9A	29.5(14)	24.6(15)	34.2(16)	13.5(13)	9.3(12)	6.9(11)
C10A	27.7(14)	26.8(16)	40.0(17)	18.8(14)	8.0(12)	8.5(11)
O1C	23.9(10)	38.3(12)	66.6(15)	32.7(11)	19.3(10)	13.0(9)
O2C	22.8(9)	26.2(11)	50.4(13)	14.9(10)	6.5(9)	10.4(8)
N1C	28.4(13)	20.7(13)	38.4(14)	11.7(12)	6.9(11)	8(1)
N2C	15.2(11)	21.8(13)	32.7(14)	12.2(11)	6.5(10)	9.4(9)
N3C	24.2(11)	21.6(13)	25.6(13)	11.4(11)	5.9(9)	10.6(10)
C1C	29.4(15)	23.7(16)	47.2(19)	18.3(15)	7.3(13)	4.1(12)
C2C	22.7(13)	23.5(15)	34.3(17)	10.4(13)	6.9(12)	3.8(11)
C3C	19.6(13)	23.6(15)	24.4(15)	8.4(12)	3.1(11)	5.2(11)
C4C	29.5(14)	28.9(16)	34.9(17)	15.7(14)	12.0(13)	9.3(12)
C5C	29.7(15)	32.7(17)	46.2(19)	19.2(15)	18.5(14)	17.9(13)
C6C	24.8(14)	25.7(16)	24.1(16)	10.8(13)	4.9(12)	9.5(12)
C7C	15.5(13)	23.0(16)	34.8(17)	12.2(13)	5.2(11)	5.6(11)
C8C	21.6(13)	24.2(16)	34.8(17)	13.4(13)	4.4(12)	4.3(11)
C9C	21.6(13)	17.7(14)	21.9(15)	6.8(12)	5.2(11)	4.5(11)
C10C	20.4(13)	23.2(15)	30.9(16)	10.3(13)	6.4(11)	3.8(11)
O1B	24.3(10)	38.3(12)	68.6(15)	34.5(12)	20.9(10)	14.6(8)
O2B	18.1(8)	18.3(10)	48.7(13)	11.8(9)	5.9(8)	8.6(7)
N1B	33.3(13)	21.4(13)	33.7(14)	9.7(11)	2.4(11)	9.5(10)
N2B	16.6(11)	26.2(13)	32.7(14)	16.8(11)	7.6(10)	10.3(9)
N3B	19.0(11)	22.1(13)	25.7(13)	10.1(10)	5.6(9)	9.3(10)
C1B	31.0(15)	34.0(18)	33.8(17)	13.0(15)	11.0(13)	13.3(13)
C2B	30.1(14)	27.1(16)	33.9(17)	17.5(14)	10.1(12)	11.9(12)
C3B	23.5(13)	17.0(15)	25.8(16)	7.8(13)	2.3(11)	4.5(11)
C4B	18.6(12)	24.8(16)	37.0(17)	12.9(14)	4.6(12)	5.2(11)
C5B	31.0(15)	19.1(15)	41.5(18)	14.0(14)	4.7(13)	0.6(12)
C6B	22.1(14)	26.2(16)	31.5(17)	15.8(14)	6.6(12)	8.2(11)
C7B	15.4(12)	28.6(17)	28.4(15)	13.6(13)	4.8(11)	7.0(11)
C8B	24.8(13)	20.6(15)	30.6(15)	9.7(12)	6.2(11)	5.6(11)
C9B	23.5(13)	19.2(14)	23.2(14)	9.6(12)	3.6(11)	1.6(10)
C10B	17.2(12)	18.7(15)	31.0(16)	11.0(12)	4.3(11)	4.1(10)
O1D	17.8(9)	33.6(12)	64.9(14)	24.9(11)	10.1(9)	8.5(8)
O2D	23.5(9)	27.4(11)	48.4(12)	15.8(10)	9.2(8)	12.4(8)
N1D	26.9(12)	27.7(14)	46.3(16)	18.8(12)	10.1(11)	12.8(10)
N2D	17.3(10)	19.7(12)	31.9(13)	10.3(10)	6.2(9)	7.7(9)
N3D	20.4(11)	19.9(13)	26.4(13)	8.9(10)	2.3(9)	7.1(10)
C1D	24.1(14)	32.5(17)	44.3(18)	18.9(14)	4.4(12)	9.4(12)
C2D	24.0(13)	23.5(15)	41.8(18)	12.4(13)	0.9(12)	0.5(11)
C3D	23.5(13)	18.3(14)	25.6(15)	9.5(12)	8.8(11)	5.4(10)
C4D	22.8(13)	25.9(16)	48.1(18)	16.8(14)	4.1(12)	4.8(11)
C5D	36.4(16)	21.1(15)	48.6(19)	12.4(14)	8.6(14)	1.5(12)
C6D	19.8(13)	18.4(15)	26.9(15)	7.1(12)	4.1(11)	2.4(11)
C7D	18.8(12)	21.8(15)	24.2(15)	4.6(12)	1.3(11)	6.8(11)
C8D	22.3(13)	18.2(15)	28.0(15)	6.0(12)	5.3(11)	2.5(10)
C9D	22.4(13)	23.9(15)	31.8(16)	12.8(13)	4.7(11)	2.5(11)
C10D	24.9(14)	23.6(15)	31.9(16)	10.8(13)	4.7(12)	9.5(11)
O1W	18.1(9)	33.4(12)	61.3(15)	15.4(11)	8.8(9)	8.0(8)
O3W	24.2(10)	50.3(14)	78.1(17)	39.9(13)	15.6(10)	10.9(9)
O2W	22.3(9)	42.2(12)	40.0(12)	14.1(10)	3.8(8)	12.3(8)

O4W	16.2(9)	40.0(12)	53.0(13)	-3.8(10)	5.7(8)	1.2(8)

Table 4 Bond Lengths for shI_3363_CoTa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1A	C6A	1.234(3)	O1B	C6B	1.230(3)
O2A	C10A	1.410(3)	O2B	C10B	1.416(3)
N1A	C1A	1.327(3)	N1B	C1B	1.341(3)
N1A	C5A	1.344(3)	N1B	C5B	1.343(3)
N2A	N3A	1.394(3)	N2B	N3B	1.390(3)
N2A	C6A	1.334(3)	N2B	C6B	1.329(3)
N3A	C7A	1.273(3)	N3B	C7B	1.268(3)
C1A	C2A	1.389(3)	C1B	C2B	1.385(4)
C2A	C3A	1.384(3)	C2B	C3B	1.387(4)
C3A	C4A	1.386(4)	C3B	C4B	1.377(3)
C3A	C6A	1.504(3)	C3B	C6B	1.518(3)
C4A	C5A	1.374(3)	C4B	C5B	1.372(4)
C7A	C8A	1.483(3)	C7B	C8B	1.483(3)
C8A	C9A	1.527(3)	C8B	C9B	1.532(3)
C9A	C10A	1.513(3)	C9B	C10B	1.521(3)
O1C	C6C	1.221(3)	O1D	C6D	1.224(3)
O2C	C10C	1.434(3)	O2D	C10D	1.424(3)
N1C	C1C	1.336(3)	N1D	C1D	1.328(4)
N1C	C5C	1.323(3)	N1D	C5D	1.345(3)
N2C	N3C	1.396(3)	N2D	N3D	1.396(3)
N2C	C6C	1.352(3)	N2D	C6D	1.338(3)
N3C	C7C	1.273(3)	N3D	C7D	1.276(3)
C1C	C2C	1.368(4)	C1D	C2D	1.380(3)
C2C	C3C	1.389(4)	C2D	C3D	1.386(3)
C3C	C4C	1.391(3)	C3D	C4D	1.382(4)
C3C	C6C	1.502(4)	C3D	C6D	1.504(3)
C4C	C5C	1.379(4)	C4D	C5D	1.383(4)
C7C	C8C	1.492(3)	C7D	C8D	1.478(3)
C8C	C9C	1.517(3)	C8D	C9D	1.518(3)
C9C	C10C	1.506(3)	C9D	C10D	1.504(3)

Table 5 Bond Angles for shI_3363_CoTa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1A	N1A	C5A	116.6(2)	C1B	N1B	C5B	116.0(2)
C6A	N2A	N3A	118.22(19)	C6B	N2B	N3B	118.64(19)
C7A	N3A	N2A	115.4(2)	C7B	N3B	N2B	115.4(2)
N1A	C1A	C2A	123.7(2)	N1B	C1B	C2B	124.1(2)
C3A	C2A	C1A	119.0(2)	C1B	C2B	C3B	118.4(3)
C2A	C3A	C4A	117.7(2)	C2B	C3B	C6B	123.6(2)
C2A	C3A	C6A	124.2(2)	C4B	C3B	C2B	118.2(2)
C4A	C3A	C6A	118.1(2)	C4B	C3B	C6B	118.2(2)
C5A	C4A	C3A	119.2(2)	C5B	C4B	C3B	119.5(2)

N1A	C5A	C4A	123.8(2)	N1B	C5B	C4B	123.8(3)
O1A	C6A	N2A	123.9(2)	O1B	C6B	N2B	123.7(2)
O1A	C6A	C3A	119.3(2)	O1B	C6B	C3B	119.2(2)
N2A	C6A	C3A	116.8(2)	N2B	C6B	C3B	117.1(2)
N3A	C7A	C8A	120.4(2)	N3B	C7B	C8B	121.6(2)
C7A	C8A	C9A	115.3(2)	C7B	C8B	C9B	114.4(2)
C10A	C9A	C8A	112.1(2)	C10B	C9B	C8B	112.4(2)
O2A	C10A	C9A	108.5(2)	O2B	C10B	C9B	107.91(19)
C5C	N1C	C1C	116.8(2)	C1D	N1D	C5D	117.1(2)
C6C	N2C	N3C	117.20(19)	C6D	N2D	N3D	118.41(19)
C7C	N3C	N2C	115.0(2)	C7D	N3D	N2D	114.83(19)
N1C	C1C	C2C	123.3(3)	N1D	C1D	C2D	123.8(2)
C1C	C2C	C3C	119.9(2)	C1D	C2D	C3D	118.8(3)
C2C	C3C	C4C	116.9(2)	C2D	C3D	C6D	123.9(2)
C2C	C3C	C6C	117.7(2)	C4D	C3D	C2D	118.2(2)
C4C	C3C	C6C	125.4(2)	C4D	C3D	C6D	117.9(2)
C5C	C4C	C3C	118.9(3)	C3D	C4D	C5D	119.0(2)
N1C	C5C	C4C	124.1(2)	N1D	C5D	C4D	123.0(3)
O1C	C6C	N2C	123.1(2)	O1D	C6D	N2D	124.8(2)
O1C	C6C	C3C	120.3(2)	O1D	C6D	C3D	119.8(2)
N2C	C6C	C3C	116.6(2)	N2D	C6D	C3D	115.4(2)
N3C	C7C	C8C	120.8(2)	N3D	C7D	C8D	120.2(2)
C7C	C8C	C9C	115.3(2)	C7D	C8D	C9D	115.7(2)
C10C	C9C	C8C	112.5(2)	C10D	C9D	C8D	111.1(2)
O2C	C10C	C9C	107.8(2)	O2D	C10D	C9D	109.5(2)

Table 6 Hydrogen Bonds for shI_3363_CoTa.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O2A	H2A	N1A[1]	0.82	2.07	2.882(3)	174.0
N2A	H2AA	O4W	0.86	1.99	2.809(3)	159.7
O2C	H2C	N1C[2]	0.82	2.00	2.816(3)	176.5
N2C	H2CA	O1W	0.86	2.00	2.833(3)	162.9
O2B	H2B	N1B[1]	0.82	1.97	2.792(3)	179.0
N2B	H2BA	O3W[3]	0.86	2.04	2.869(3)	162.8
O2D	H2D	N1D[1]	0.85	1.98	2.791(2)	158.7
N2D	H2DA	O2W	0.86	2.03	2.821(2)	152.5
O1W	H1WA	O2D[3]	0.85	2.00	2.838(3)	170.1
O1W	H1WB	O1C[4]	0.85	2.16	2.873(2)	141.8
O1W	H1WB	N3C[4]	0.85	2.54	3.275(3)	144.5
O3W	H3WA	O1A	0.85	2.45	3.293(3)	171.3
O3W	H3WB	O1B	0.85	1.99	2.814(3)	163.9
O3W	H3WB	N3B	0.85	2.69	3.256(3)	125.6
O2W	H2WA	O1D[3]	0.85	2.03	2.850(2)	161.4
O2W	H2WB	O2C[4]	0.85	1.97	2.819(3)	174.1
O4W	H4WA	O1A[3]	0.85	2.00	2.831(2)	167.3
O4W	H4WB	O2B[3]	0.86	1.97	2.768(3)	153.5

[1]1+X,-1+Y,+Z; [2]-1+X,1+Y,+Z; [3]-1+X,+Y,+Z; [4]1+X,+Y,+Z

Table 7 Torsion Angles for shI_3363_CoTa.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1A	C1A	C2A	C3A	1.2(4)	N1B	C1B	C2B	C3B	0.8(5)
N2A	**N3A**	**C7A**	**C8A**	-178.6(2)	N2B	N3B	C7B	C8B	178.1(2)
N3A	N2A	C6A	O1A	2.4(4)	N3B	N2B	C6B	O1B	1.3(4)
N3A	**N2A**	**C6A**	**C3A**	-176.8(2)	N3B	N2B	C6B	C3B	178.8(2)
N3A	C7A	C8A	C9A	1.2(4)	N3B	C7B	C8B	C9B	3.1(4)
C1A	N1A	C5A	C4A	0.0(4)	C1B	N1B	C5B	C4B	-0.6(4)
C1A	C2A	C3A	C4A	-1.0(4)	C1B	C2B	C3B	C4B	0.1(4)
C1A	C2A	C3A	C6A	176.5(2)	C1B	C2B	C3B	C6B	178.9(3)
C2A	C3A	C4A	C5A	0.4(4)	C2B	C3B	C4B	C5B	-1.2(4)
C2A	C3A	C6A	O1A	-160.3(2)	C2B	C3B	C6B	O1B	-161.3(3)
C2A	C3A	C6A	N2A	18.9(4)	C2B	C3B	C6B	N2B	21.1(4)
C3A	C4A	C5A	N1A	0.2(4)	C3B	C4B	C5B	N1B	1.5(4)
C4A	C3A	C6A	O1A	17.2(4)	C4B	C3B	C6B	O1B	17.5(4)
C4A	C3A	C6A	N2A	-163.6(2)	C4B	C3B	C6B	N2B	-160.1(2)
C5A	N1A	C1A	C2A	-0.7(4)	C5B	N1B	C1B	C2B	-0.6(4)
C6A	**N2A**	**N3A**	**C7A**	-178.3(2)	C6B	N2B	N3B	C7B	-165.7(2)
C6A	C3A	C4A	C5A	-177.3(2)	C6B	C3B	C4B	C5B	180.0(3)
C7A	C8A	C9A	C10A	167.5(2)	C7B	C8B	C9B	C10B	-176.5(2)
C8A	C9A	C10A	O2A	178.8(2)	C8B	C9B	C10B	O2B	-178.0(2)
N1C	C1C	C2C	C3C	-1.4(4)	N1D	C1D	C2D	C3D	-1.4(4)
N2C	N3C	C7C	C8C	-179.8(2)	N2D	N3D	C7D	C8D	-177.6(2)
N3C	N2C	C6C	O1C	0.3(4)	N3D	N2D	C6D	O1D	0.0(4)
N3C	N2C	C6C	C3C	-180.0(2)	N3D	N2D	C6D	C3D	179.6(2)
N3C	C7C	C8C	C9C	-4.8(4)	N3D	C7D	C8D	C9D	-3.2(4)
C1C	N1C	C5C	C4C	-0.6(4)	C1D	N1D	C5D	C4D	0.3(4)
C1C	C2C	C3C	C4C	1.0(4)	C1D	C2D	C3D	C4D	0.3(4)
C1C	C2C	C3C	C6C	179.1(3)	C1D	C2D	C3D	C6D	-177.6(2)
C2C	C3C	C4C	C5C	-0.5(4)	C2D	C3D	C4D	C5D	1.0(4)
C2C	C3C	C6C	O1C	-18.8(4)	C2D	C3D	C6D	O1D	152.5(3)
C2C	C3C	C6C	N2C	161.5(2)	C2D	C3D	C6D	N2D	-27.1(4)
C3C	C4C	C5C	N1C	0.3(5)	C3D	C4D	C5D	N1D	-1.4(4)
C4C	C3C	C6C	O1C	159.1(3)	C4D	C3D	C6D	O1D	-25.4(4)
C4C	C3C	C6C	N2C	-20.6(4)	C4D	C3D	C6D	N2D	155.1(2)
C5C	N1C	C1C	C2C	1.1(4)	C5D	N1D	C1D	C2D	1.2(4)
C6C	N2C	N3C	C7C	173.2(2)	C6D	N2D	N3D	C7D	176.2(2)
C6C	C3C	C4C	C5C	-178.5(3)	C6D	C3D	C4D	C5D	179.0(2)
C7C	C8C	C9C	C10C	173.0(2)	C7D	C8D	C9D	C10D	-178.2(2)
C8C	C9C	C10C	O2C	177.5(2)	C8D	C9D	C10D	O2D	-168.8(2)

Table 8 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for shI_3363_CoTa.

Atom	*x*	*y*	*z*	U(eq)
H2A	15544	6814	14035	68

H2AA	7321	11055	13617	24
H1A	4343	14344	14252	30
H2AB	5882	12641	14134	29
H4A	10658	14007	13374	30
H5A	8952	15638	13487	33
H7A	7217	9203	13520	29
H8AA	9102	7490	13016	29
H8AB	9232	7945	14140	29
H9AA	12394	8295	13175	34
H9AB	12517	9025	14284	34
H10A	12538	7260	14599	35
H10B	12367	6516	13486	35
H2C	-4291	10681	8751	49
H2CA	3707	6132	8643	27
H1C	2301	1975	9508	38
H2CB	636	3576	9490	32
H4C	4929	4409	8156	35
H5C	6428	2755	8199	40
H7C	3851	7962	8690	29
H8CA	1833	9286	8168	31
H8CB	2147	9755	9300	31
H9CA	-1465	8461	8028	24
H9CB	-1157	8768	9150	24
H10C	-1039	10795	9425	29
H10D	-1251	10513	8305	29
H2B	13218	8071	11260	43
H2BA	5335	12662	11332	28
H1B	2503	15972	11760	38
H2BB	4069	14332	11808	33
H4B	8411	15245	10540	32
H5B	6675	16812	10486	36
H7B	5090	10765	11095	28
H8BA	6837	9011	10471	30
H8BB	6935	9364	11588	30
H9BA	10207	10002	10793	26
H9BB	10301	10274	11901	26
H10E	10088	8203	11587	26
H10F	10074	7953	10483	26
H2D	15724	4198	6197	48
H2DA	7499	8655	6114	27
H1D	4139	11366	5442	39
H2DB	5799	9749	5463	36
H4D	10960	11950	6793	38
H5D	9105	13512	6786	43
H7D	7403	6877	6165	27
H8DA	9051	5095	5685	28
H8DB	9612	5701	6815	28
H9DA	12257	5903	5562	30
H9DB	12820	6472	6698	30
H10G	12441	4486	6703	32

H10H	12312	4019	5573	32
H1WA	6012	5856	7696	57
H1WB	7603	6396	8530	57
H3WA	12393	12285	12227	68
H3WB	11505	12627	11478	68
H2WA	3950	8787	6429	53
H2WB	5250	9007	7308	53
H4WA	3483	10969	13326	64
H4WB	3498	10058	12575	64

3. Antibacterial and antifungal activity

Table 3S. The inhibition of growth for compounds **1**, **4**, **6** and **INH** against 5 bacteria: *Escherichia coli*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa* and *Staphylococcus aureus*, and 2 fungi: *Candida albicans* and *Cryptococcus neoformans*.

	1	Z-score	**1**	Z-score	**2**	Z-score	**2**	Z-score	**3**	Z-score	**3**	Z-score
	a		b		a		b		a		b	
1	10.23	0.72	10.81	0.8	6.12	0.99	4.13	1.45	5.16	1.14	2.28	0.85
4	23.11	-0.17	19.73	0.13	13.57	-0.16	10.25	0.38	24.88	-0.97	13.75	-0.63
6	30.27	-0.64	23.84	-0.17	16.51	-0.61	13.26	-0.13	26.27	-1.12	10.99	-0.27
INH	29.58	-0.63	25.18	-0.27	19.97	-1.15	21.05	-1.49	23.11	-0.78	14.53	-0.73

	4	Z-score	**4**	Z-score	**5**	Z-score	**5**	Z-score	**6**	Z-score	**6**	Z-score	**7**	Z-score
	a		b		a		b		a		b		a	
1	4,62	1.00	-2.35	1.16	5.57	0.64	1.47	0.95	-1.62	0.87	3.13	0.41	-50.92	0.31
4	26.0	-2.12	11.88	-0.96	21.62	-1.94	4.78	0.34	2.96	0.25	4.33	0.21	-64.37	0.61
6	12.36	-0.13	7.61	-0.32	12.65	-0.49	5.18	0.26	-1.88	0.91	2.31	0.54	-81.79	1.00
INH	13.45	-0.29	1.60	0.57	15.31	-0.92	9.88	-0.61	-0.35	0.70	2.31	0.54	-55.93	0.42

The compounds were tested at a concentration of 32μg/mL. All screening is performed as two replica (n=2), with both replicas on different assay plates, but from single plating and performed in a single screening experiment (microbial incubation). Each individual value is reported in the table (a and b; See protocol of CO-ACD).

Bacteria: 1 = *Staphylococcus aureus*-Strain: ATCC 43300 (1), 1b = *Staphylococcus aureus*-Strain ATCC 43300 (2); 2) *Escherichia coli*-Strain: ATCC 25922; 3) *Klebsiella pneumoniae*-Strain: ATCC 700603; 4) *Acinetobacter baumannii*-Strain: ATCC 19606; 5) *Pseudomonas aeruginosa*-Strain: ATCC 27853;
Fungi: 6) *Candida albicans*-Strain: ATCC 90028; 7) *Cryptococcus neoformans* var. grubii-Strain: H99; ATCC 208821.

4. TLC slides from experimental part

4.1. TLC of 2-HO-THF (1), THF^{X} (2), crude HOO-THF (3) and THF^{Y} in dichloromethane-methanol, 9:1, visualization with 2,4-dinitrophenylhydrazone reagent and heating at 110 ˚C for ~10 min.

1. 2-HO-THF

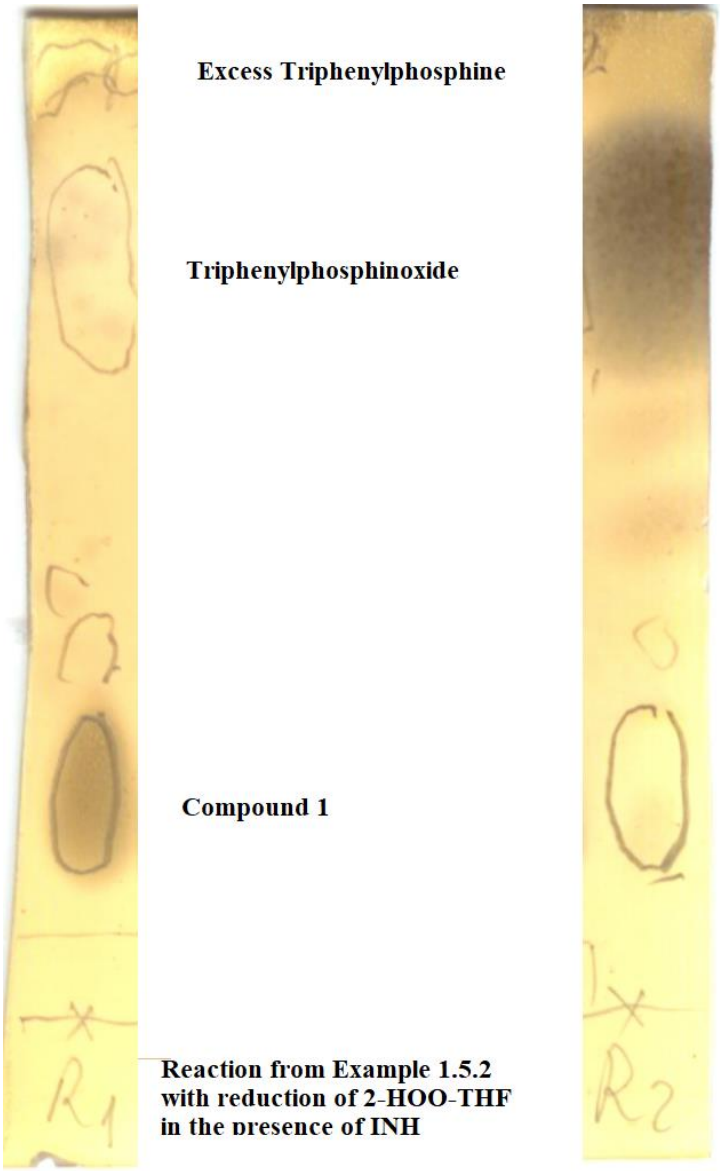
2. THFX with 2-HO-THF and 2-HOO-THF, used in the paper

3. Crude 2-HOO-THF synthesized

4. THFY with 2-HOO-THF, used in the Example 1.5.2.

4.2.TLC with the secondary compound formed in two reactions from example 1.3 (C, mother liquors after crystallization, D, TLC during reaction).

4.3. TLC of the reaction mixture of the example 1.5.2. (left, R1) and of the reaction of THF[Y] with 2-HOO-THF (wright, R2).



Reaction from Example 1.5.2 with reduction of 2-HOO-THF in the presence of INH

Reaction of HOO-THF with INH in the same conditions as for Example 1.5.2.