Supporting information for

Synthesis and Antiviral Activity of 4,6-Disubstituted Pyrimido[4,5-*b*]indole Ribonucleosides

Michal Tichý,[a] Radek Pohl,[a] Hao Ying Xu,[b] Yen-Liang Chen,[b] Fumiaki Yokokawa,[b] Pei-Yong Shi,[b] and Michal Hocek[a,c]*

[a] *Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Gilead Sciences & IOCB Research Center, Flemingovo nam. 2, CZ-16610 Prague 6, Czech Republic*

[b] *Novartis Institute for Tropical Diseases, 10 Biopolis Road, #05-01 Chromos, Singapore 138670*

[c] *Department of Organic and Nuclear Chemistry, Faculty of Science, Charles University in Prague, Hlavova 8, CZ-12843 Prague 2, Czech Republic*

Contents:

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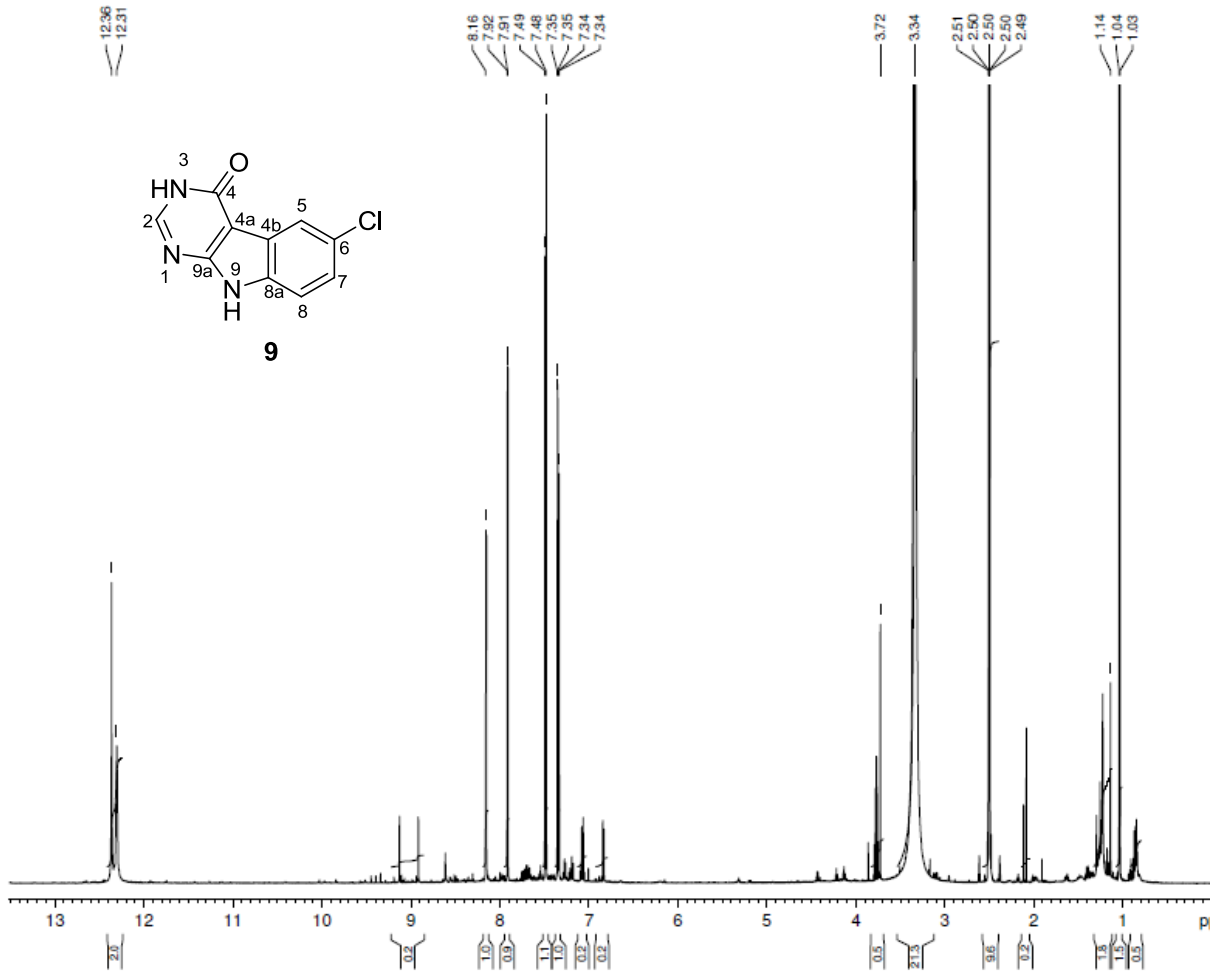
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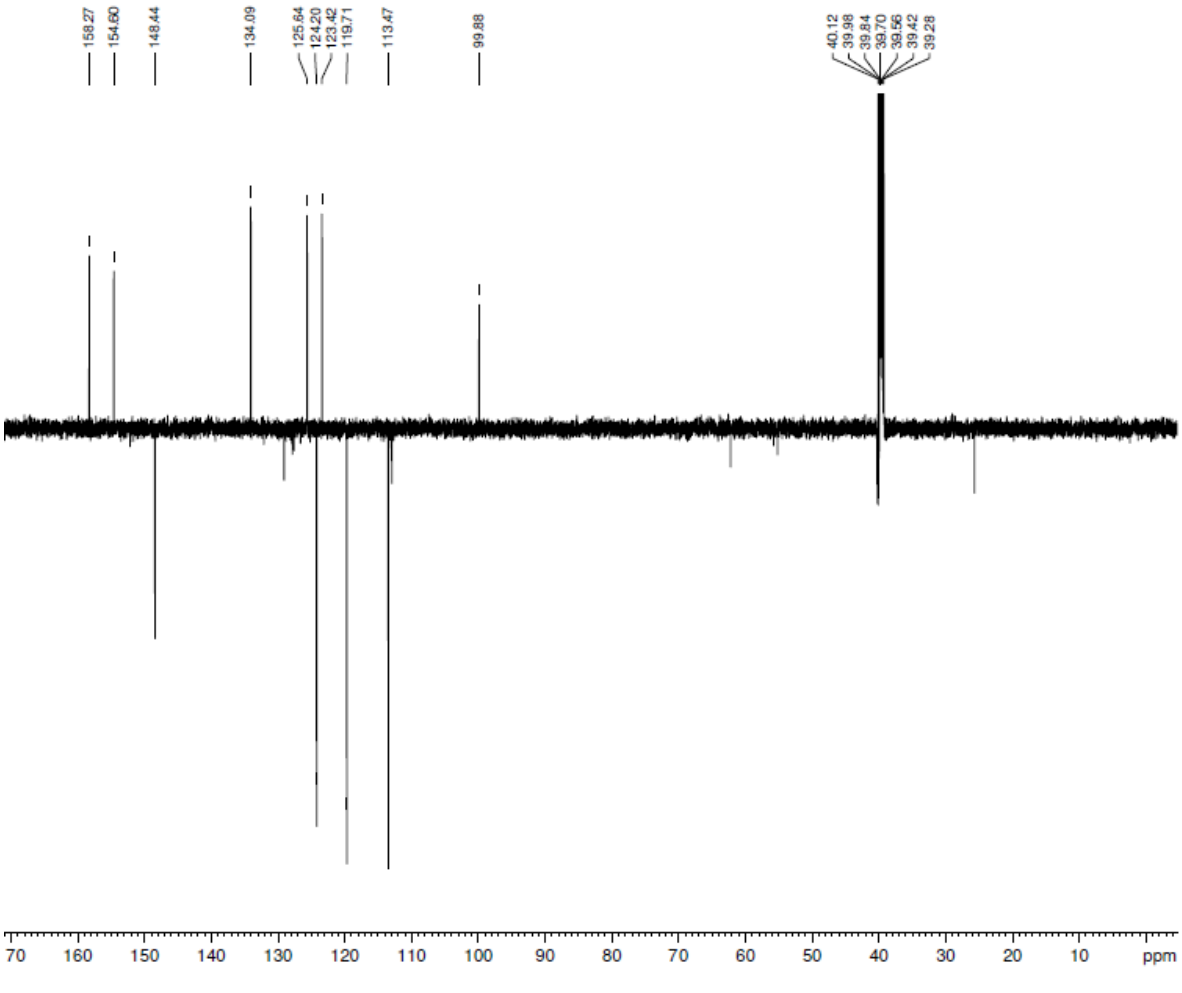
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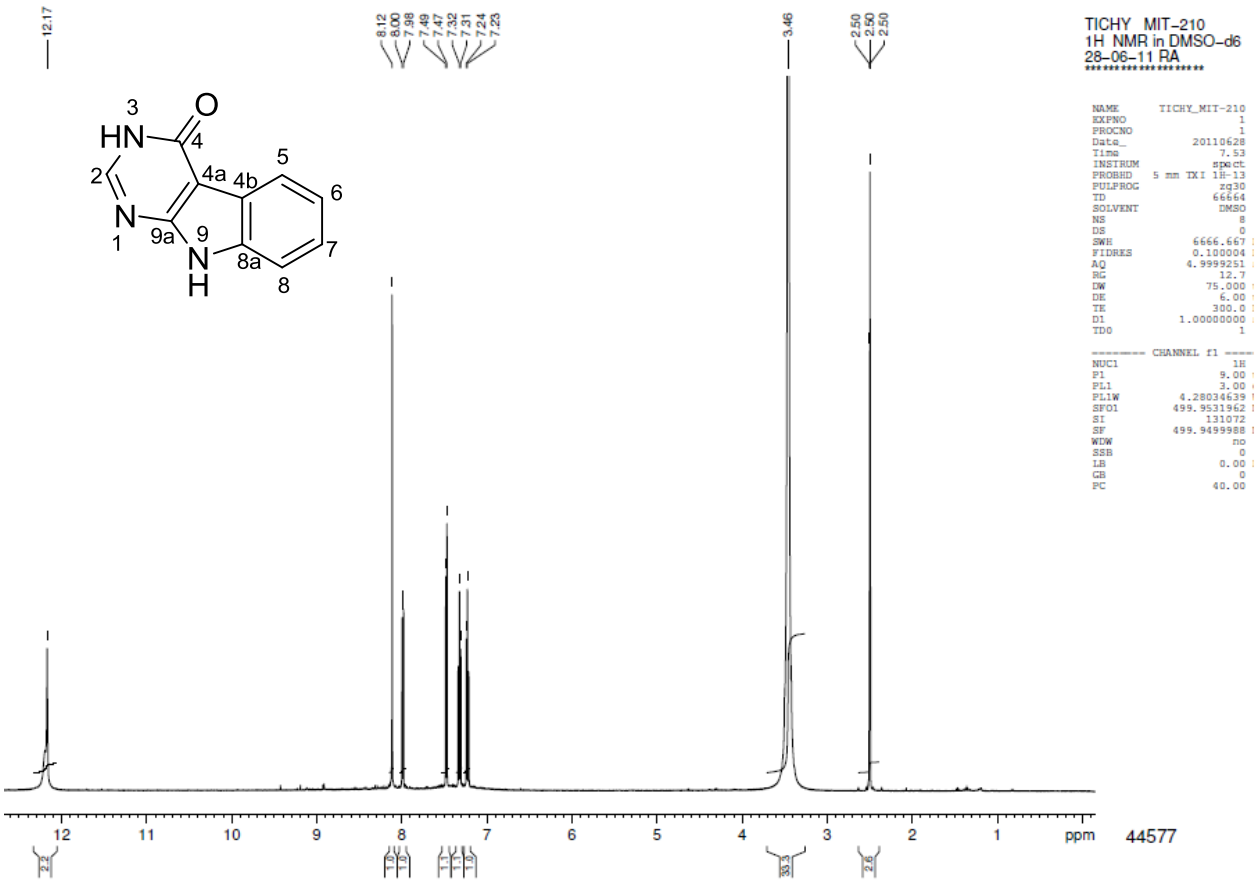
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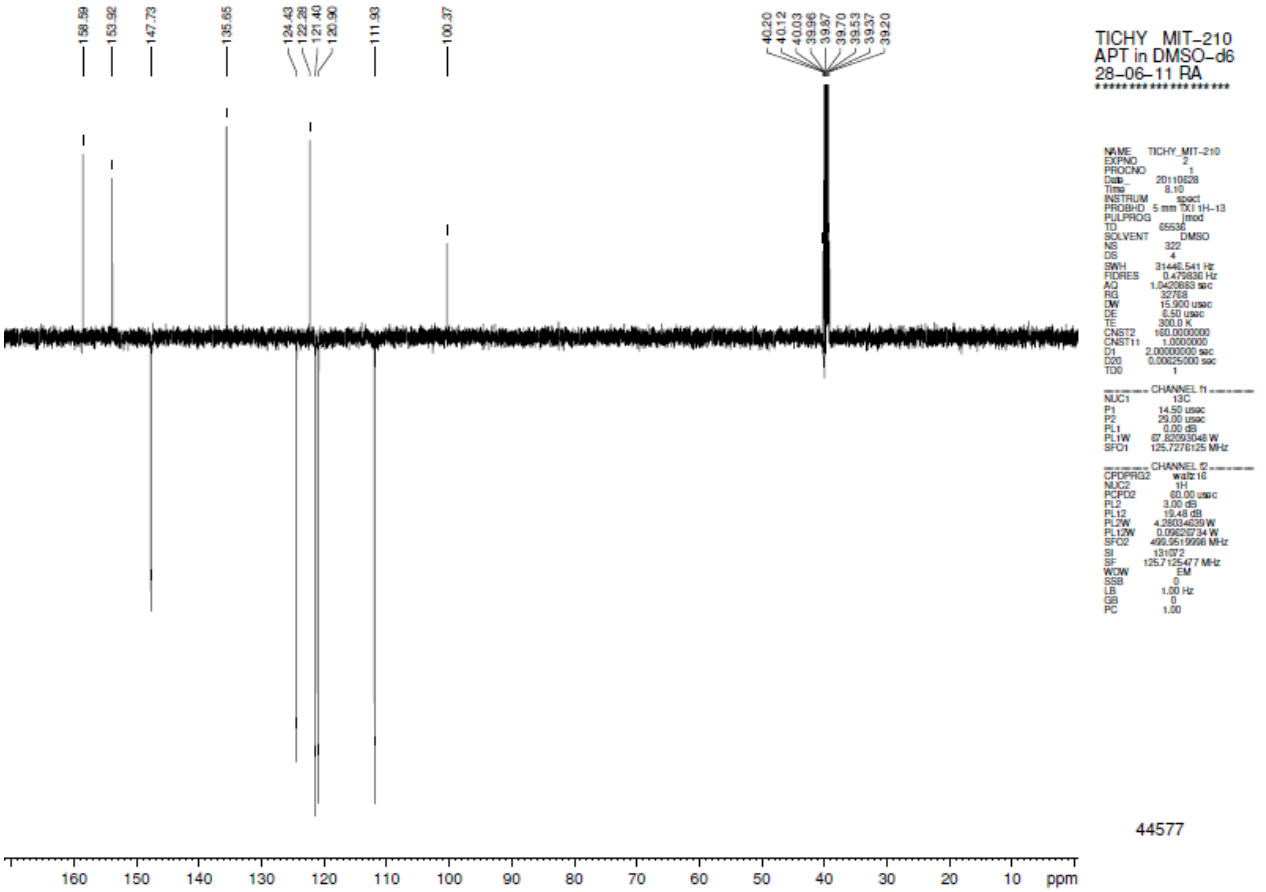
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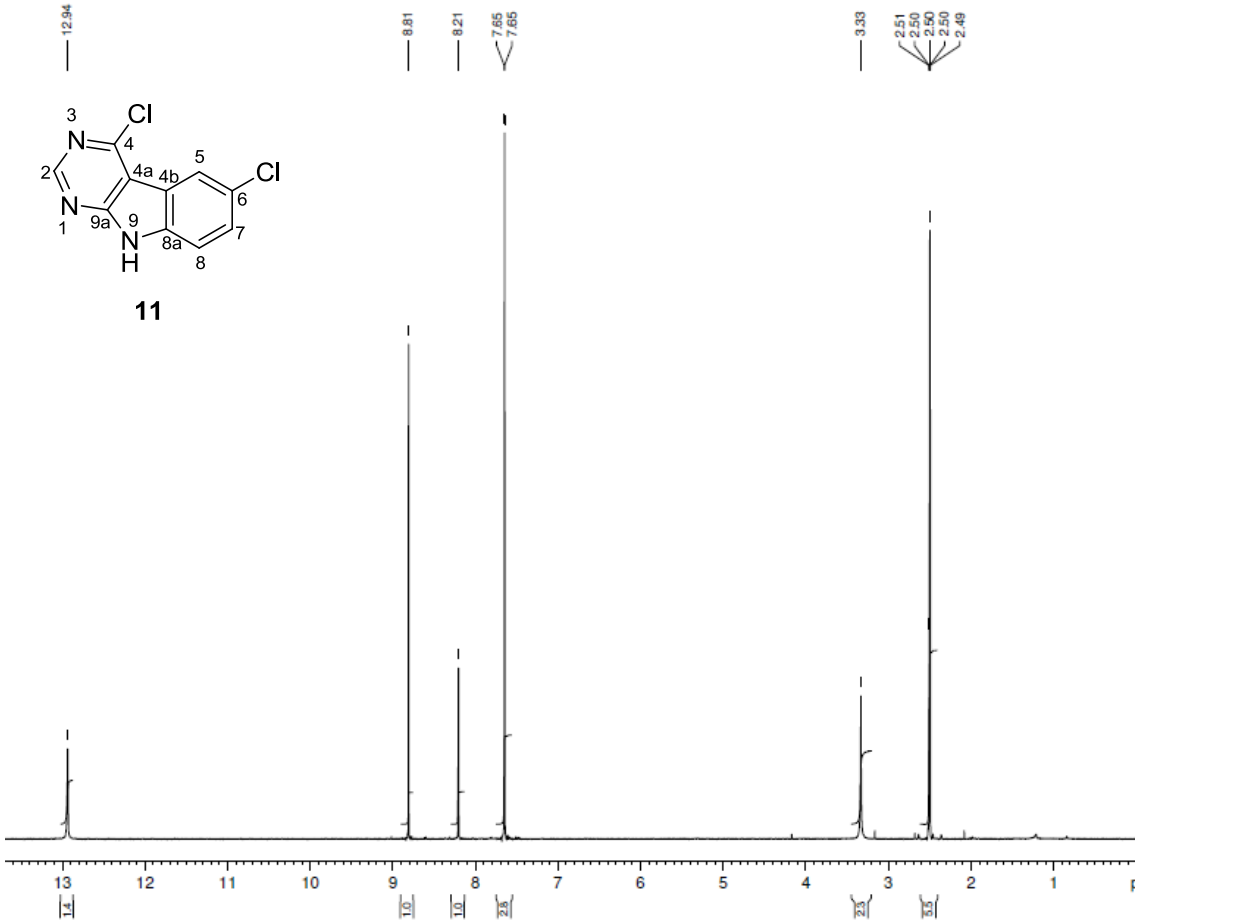
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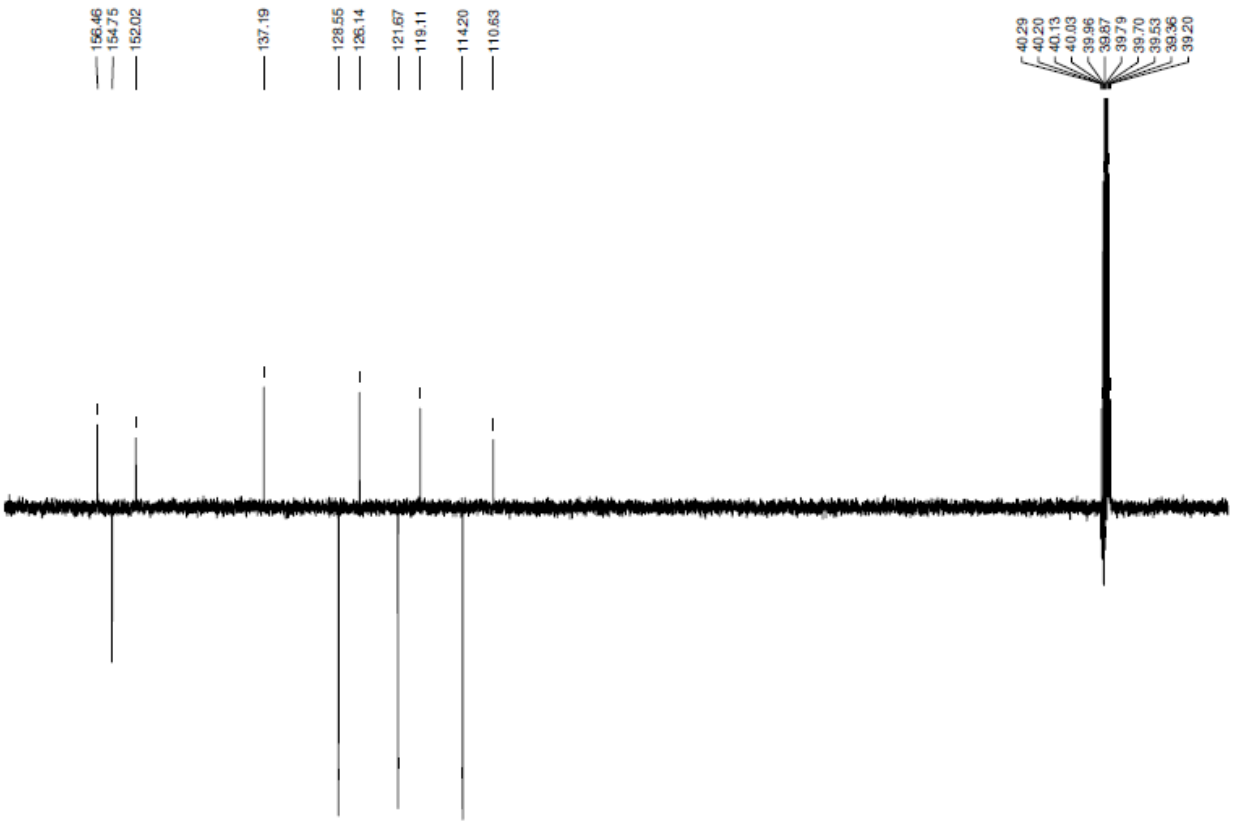
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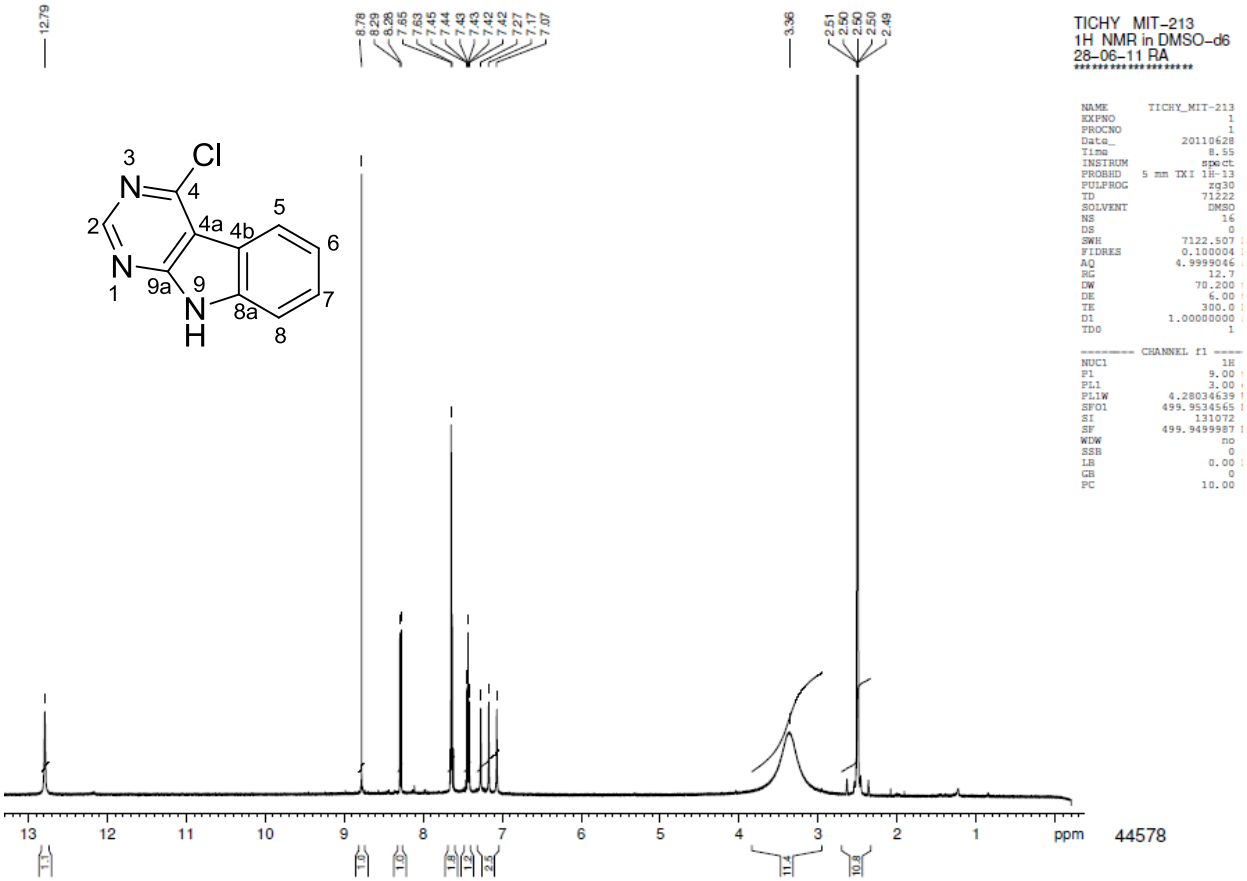
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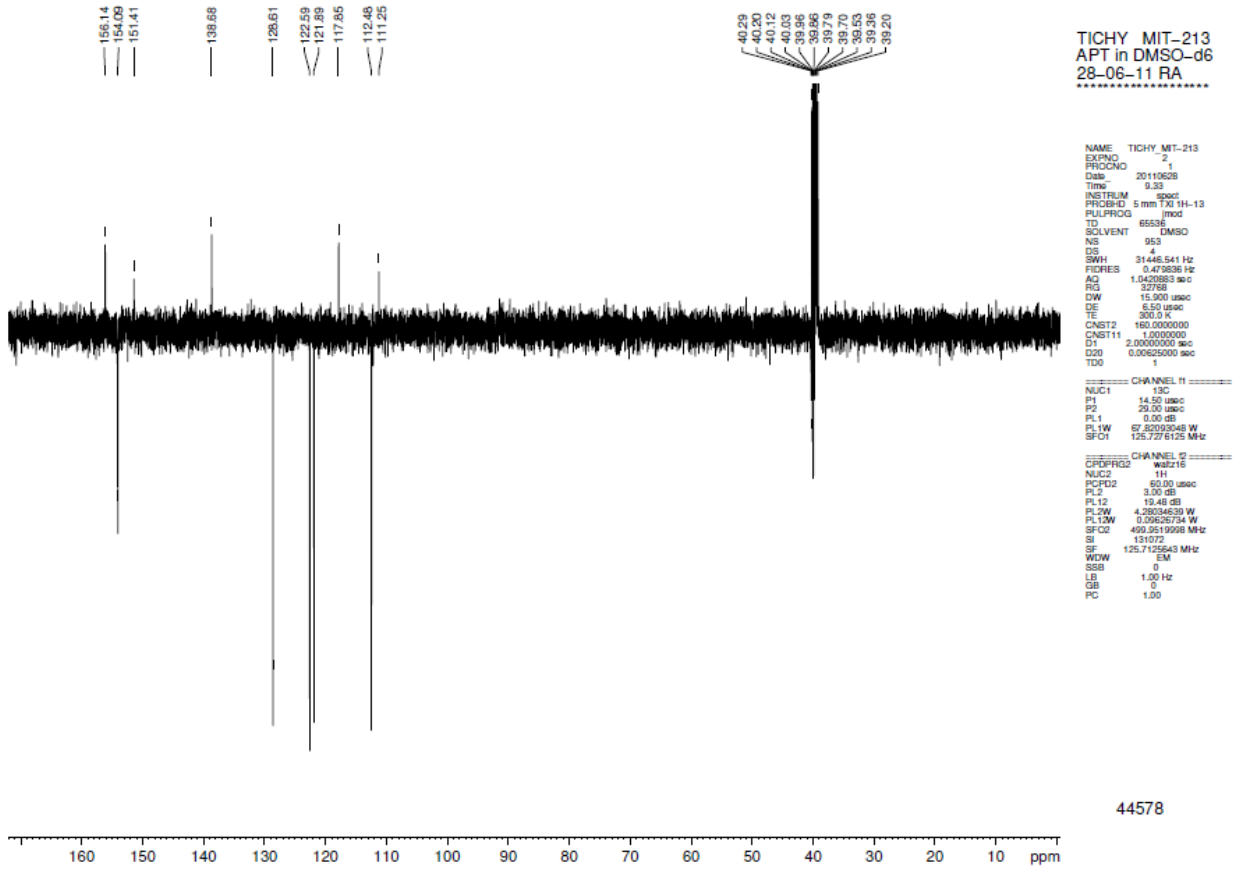
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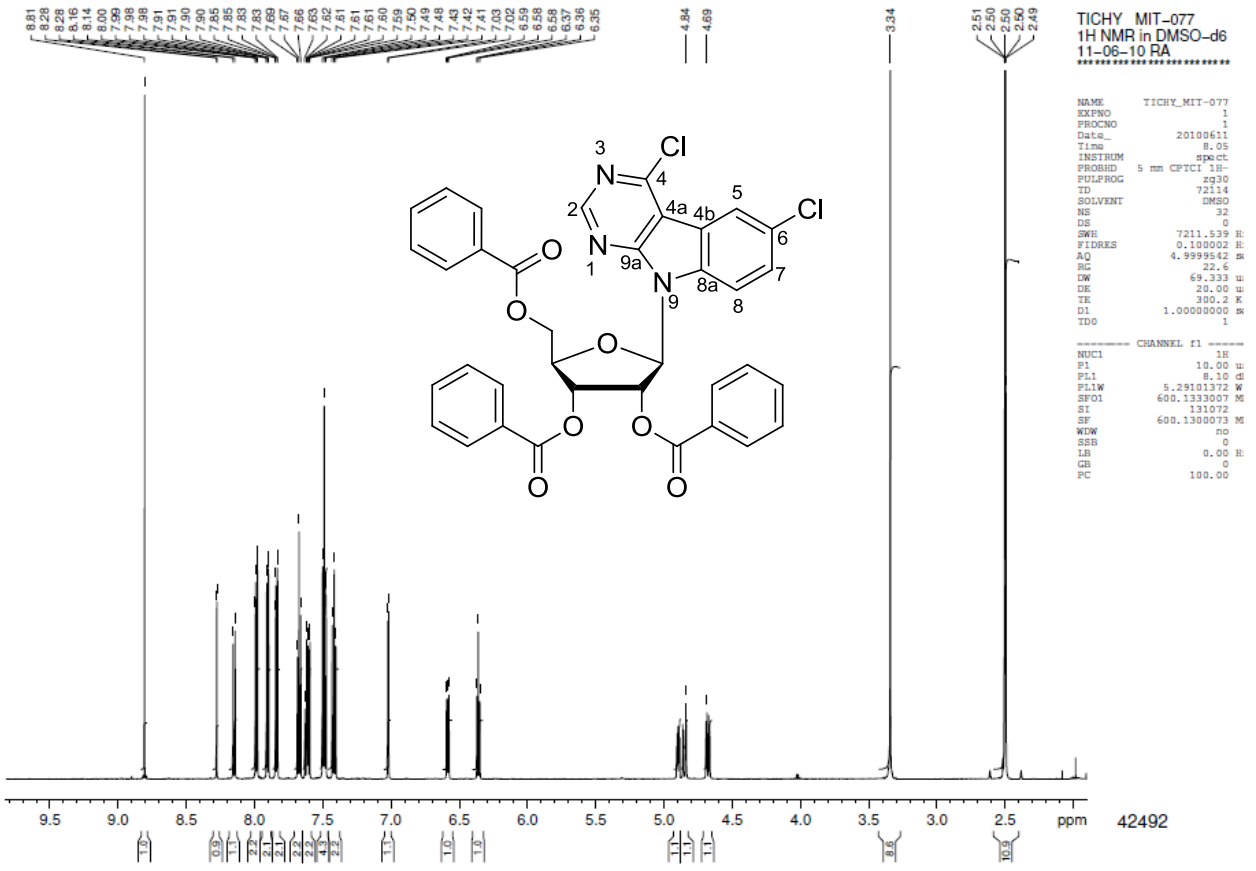
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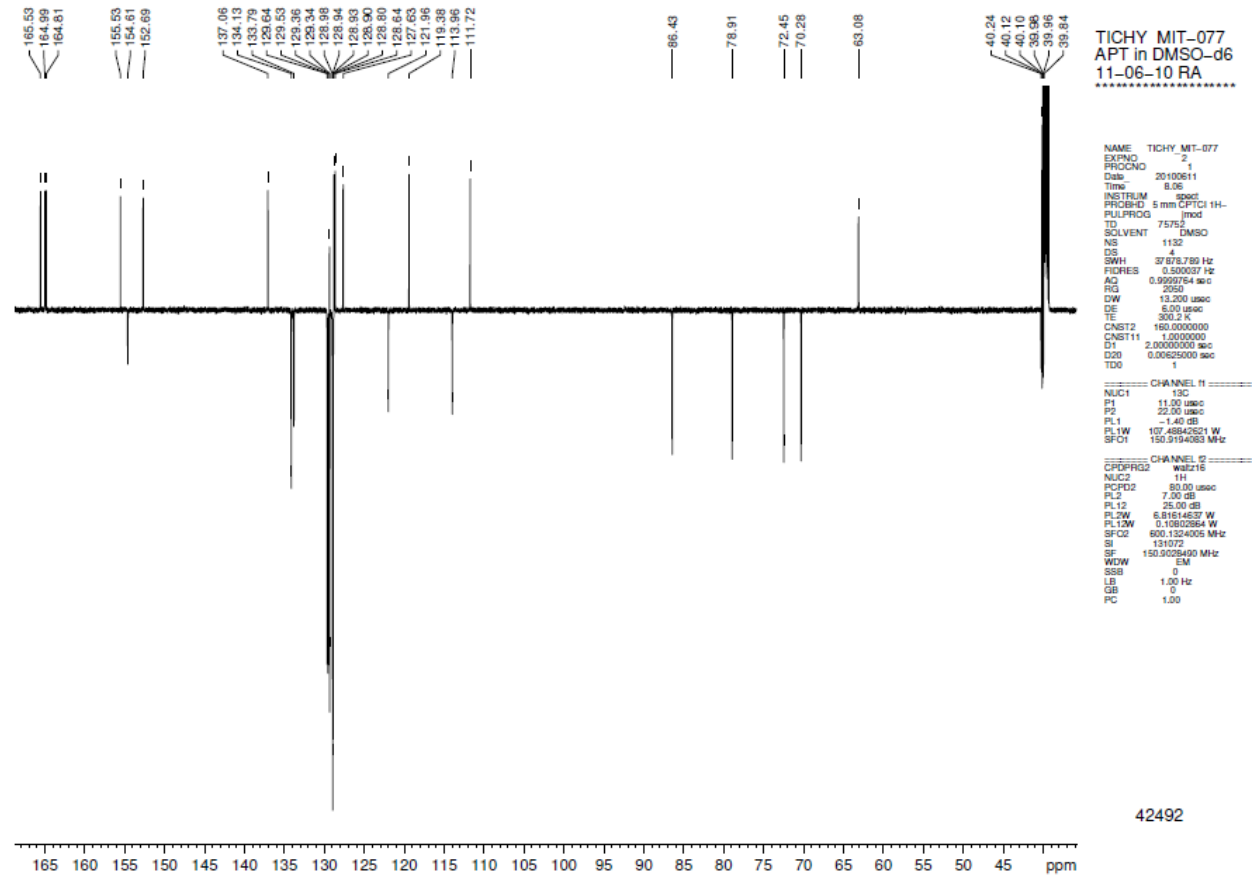
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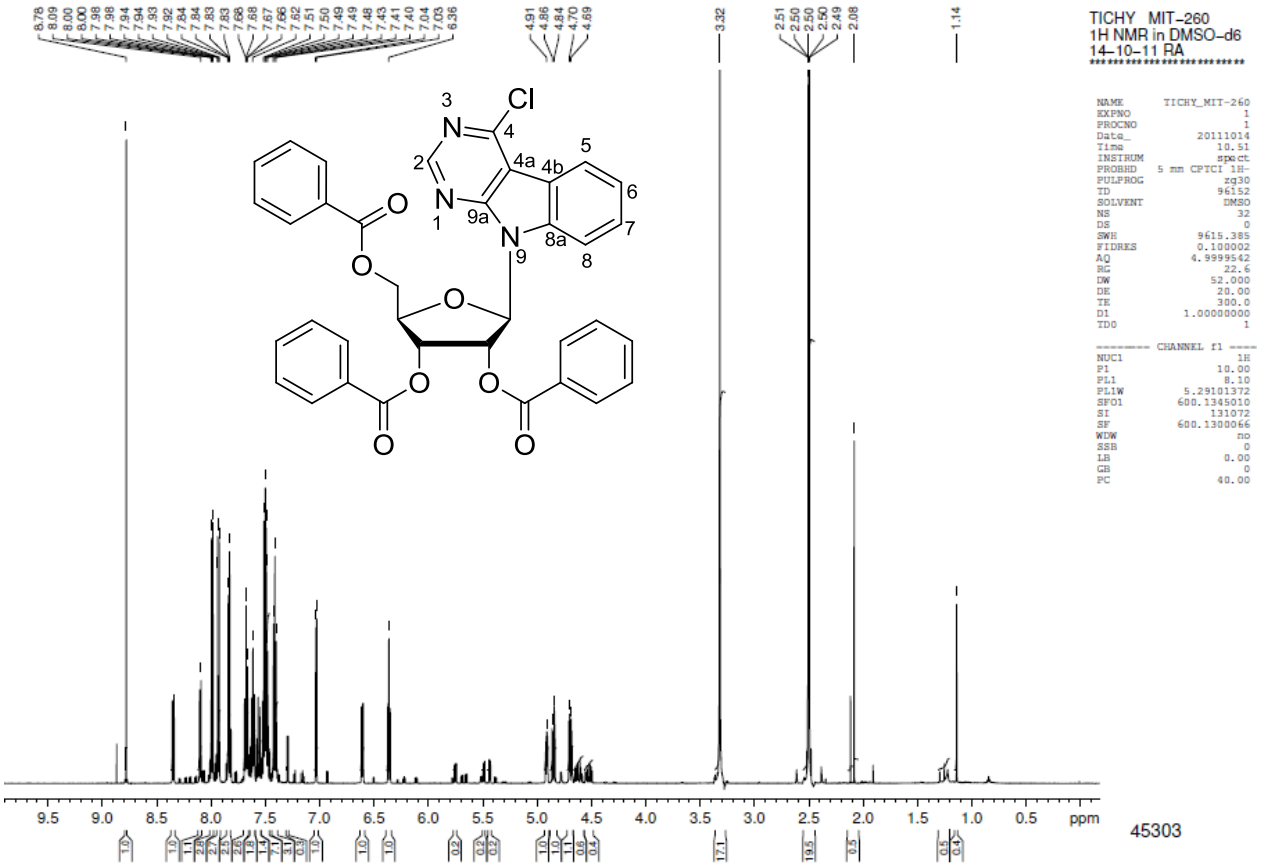
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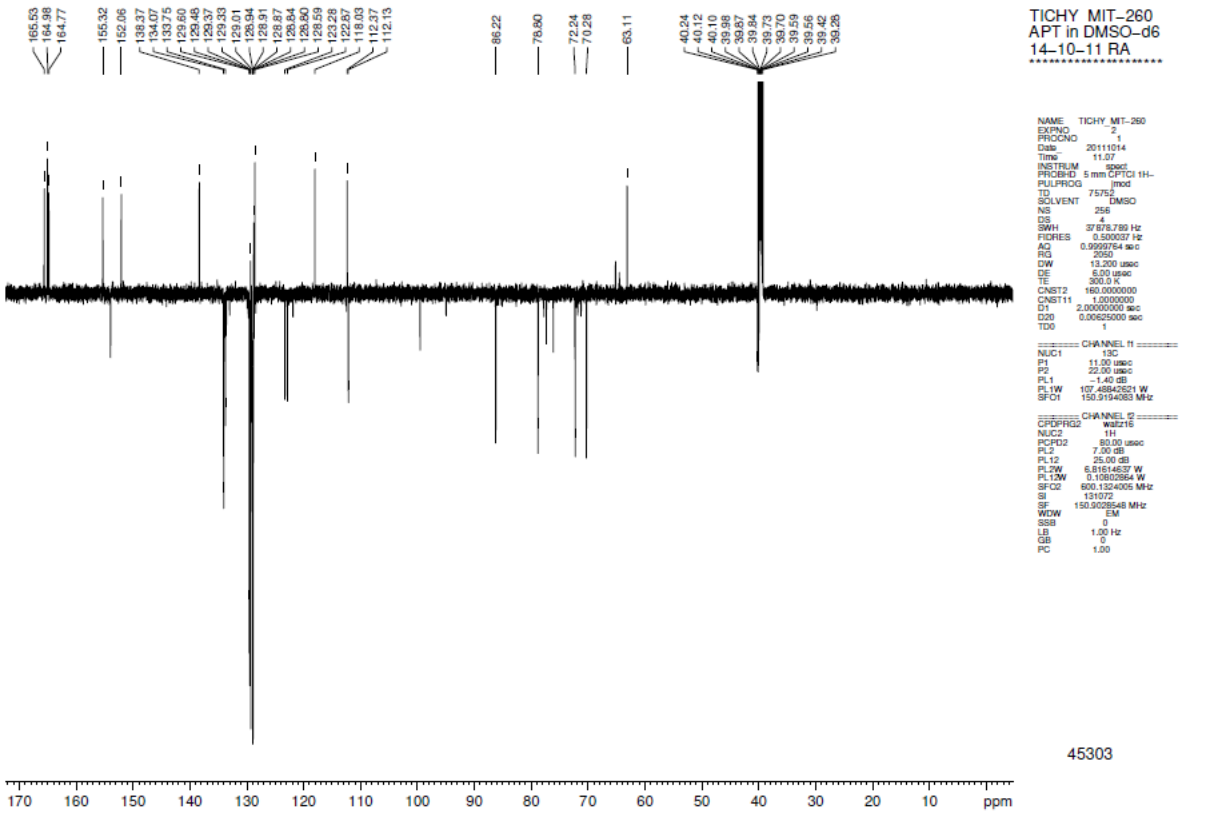
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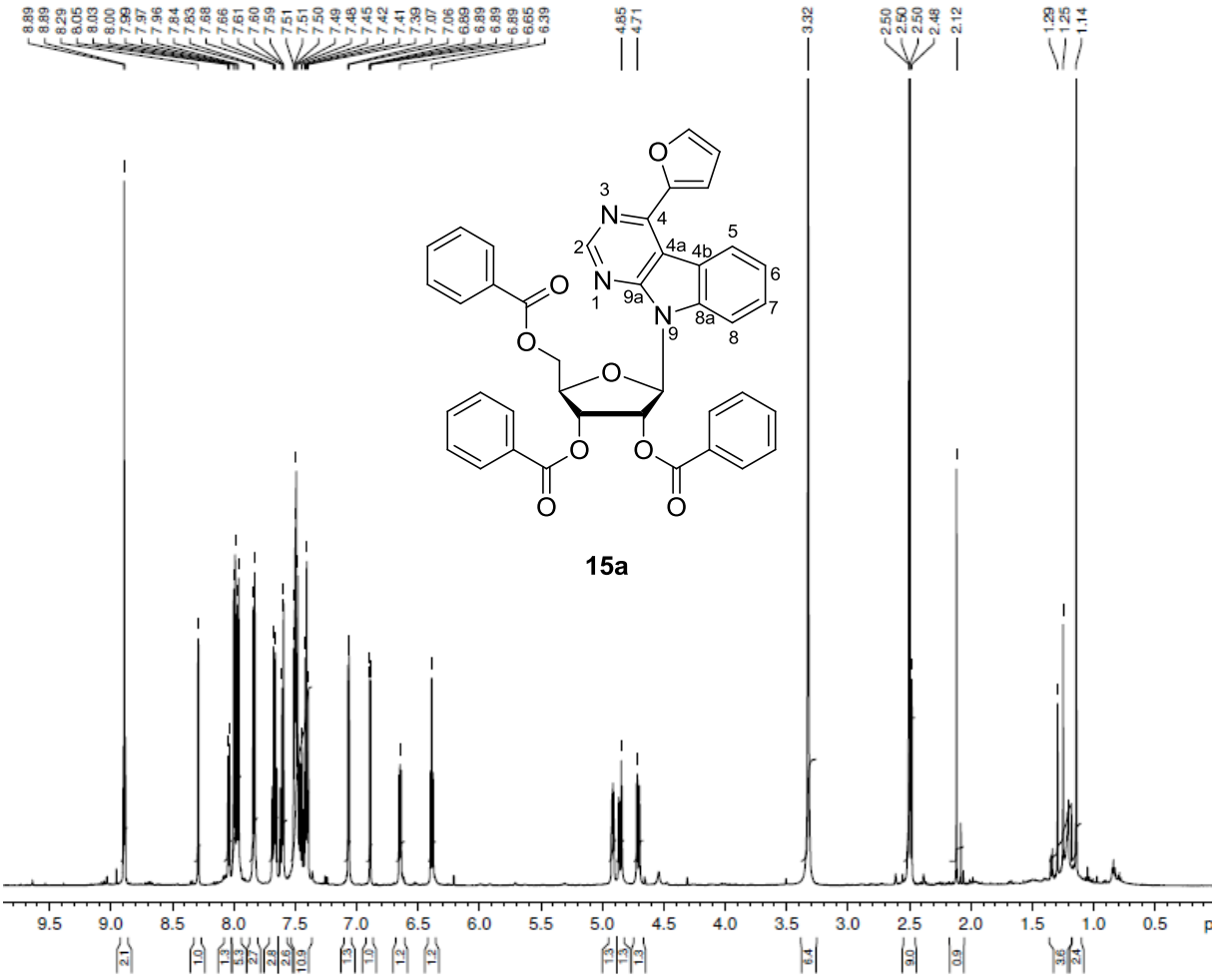
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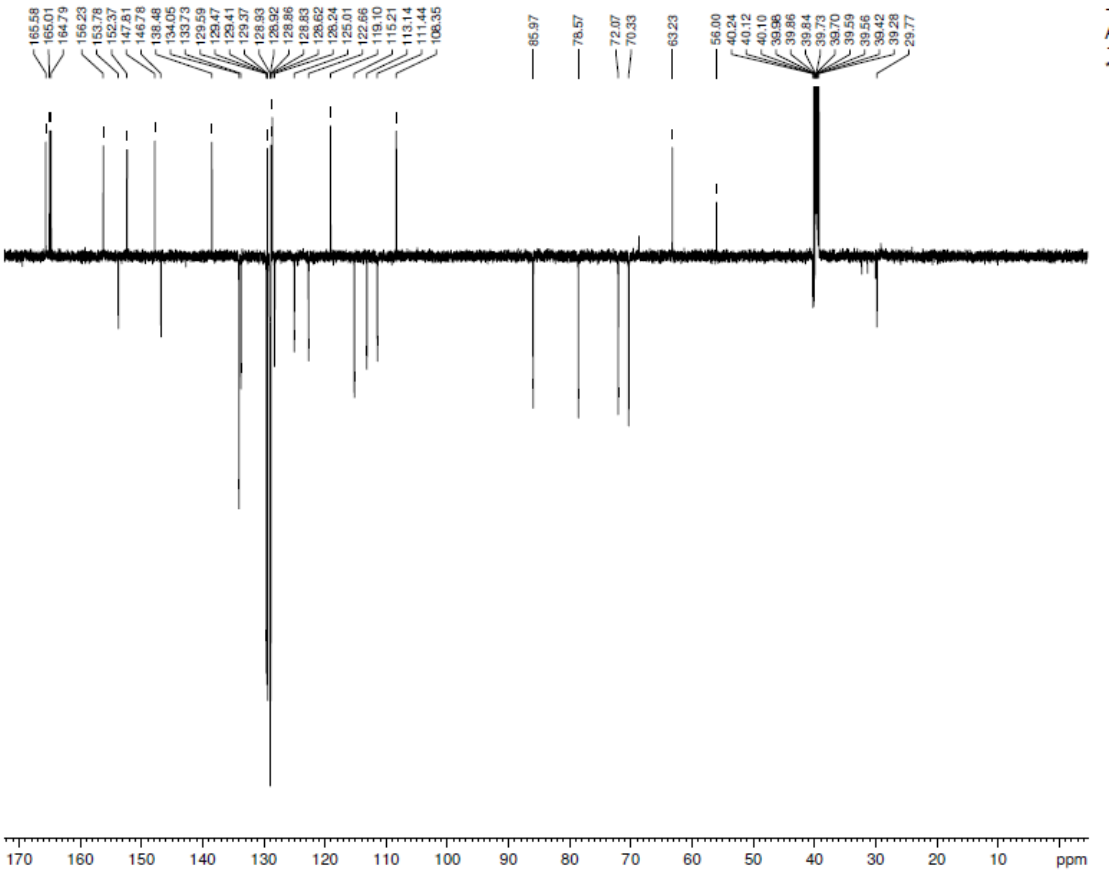
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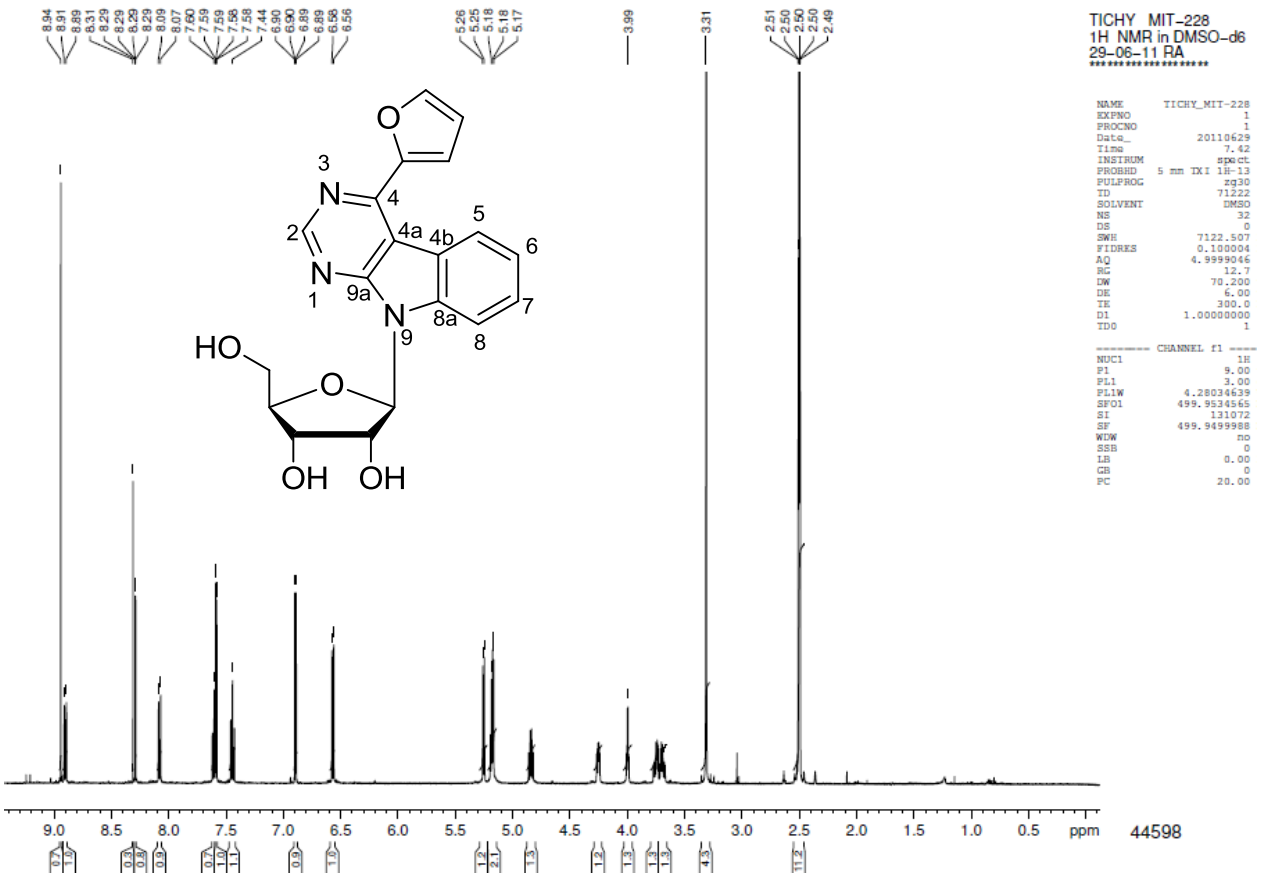
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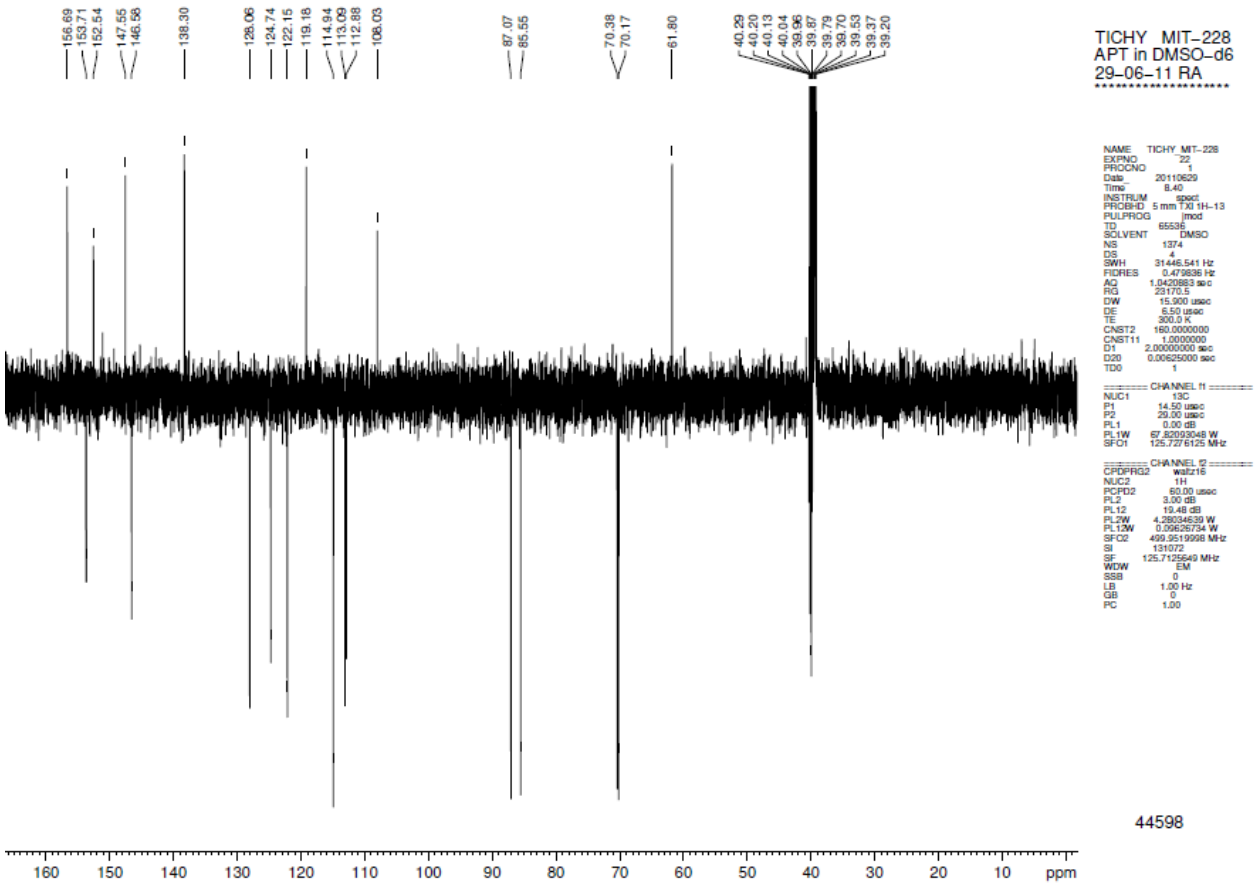
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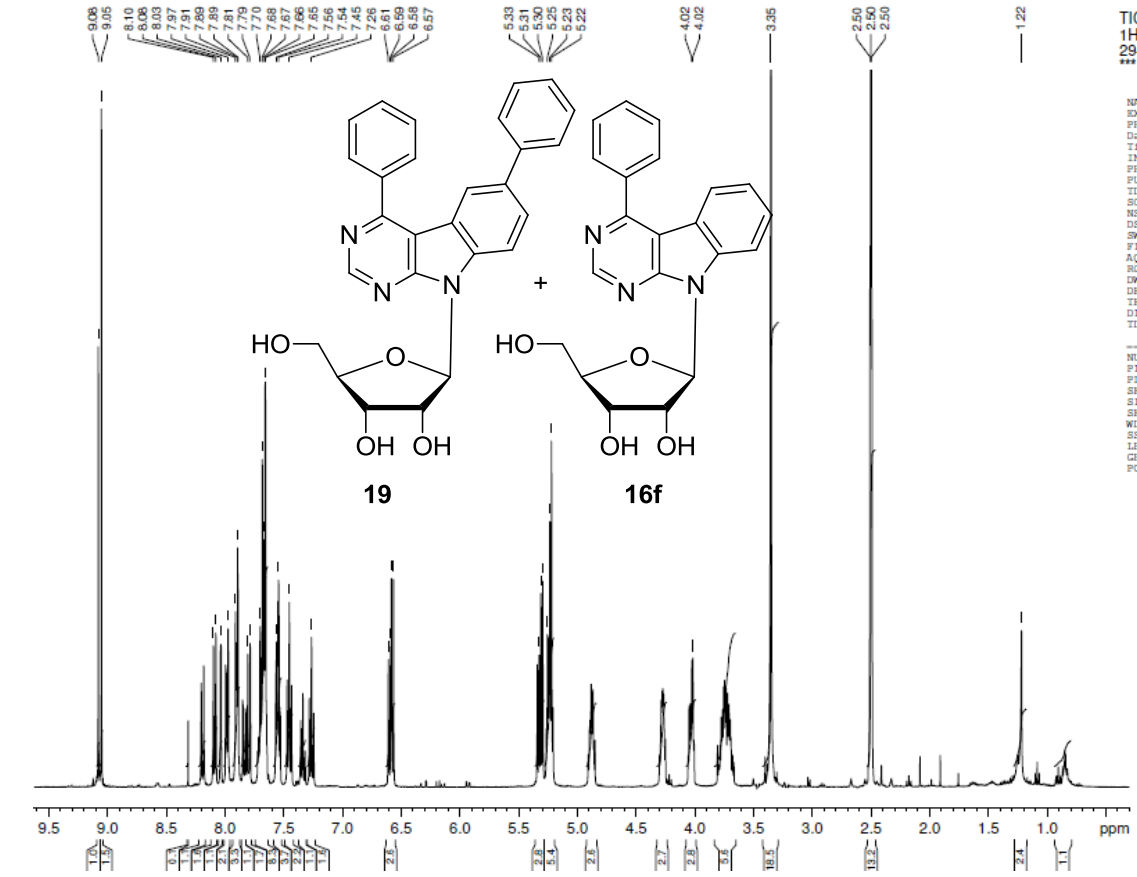
16f +19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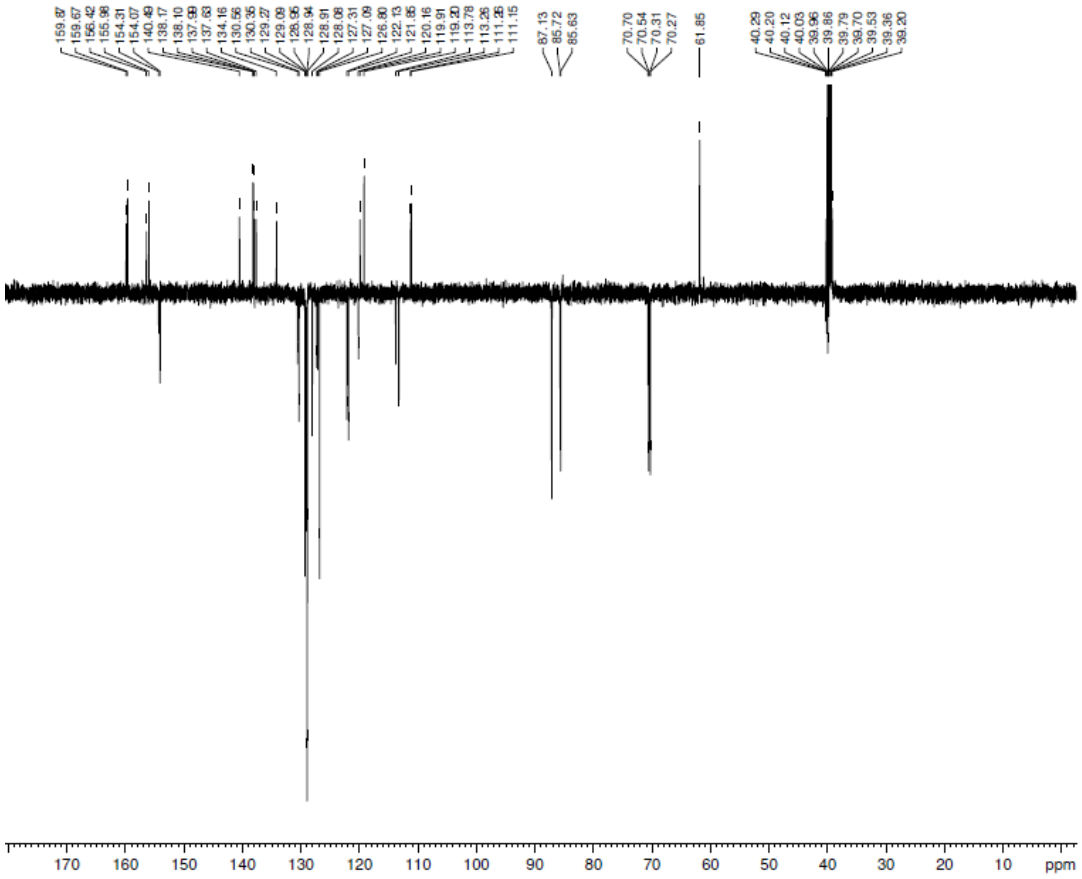
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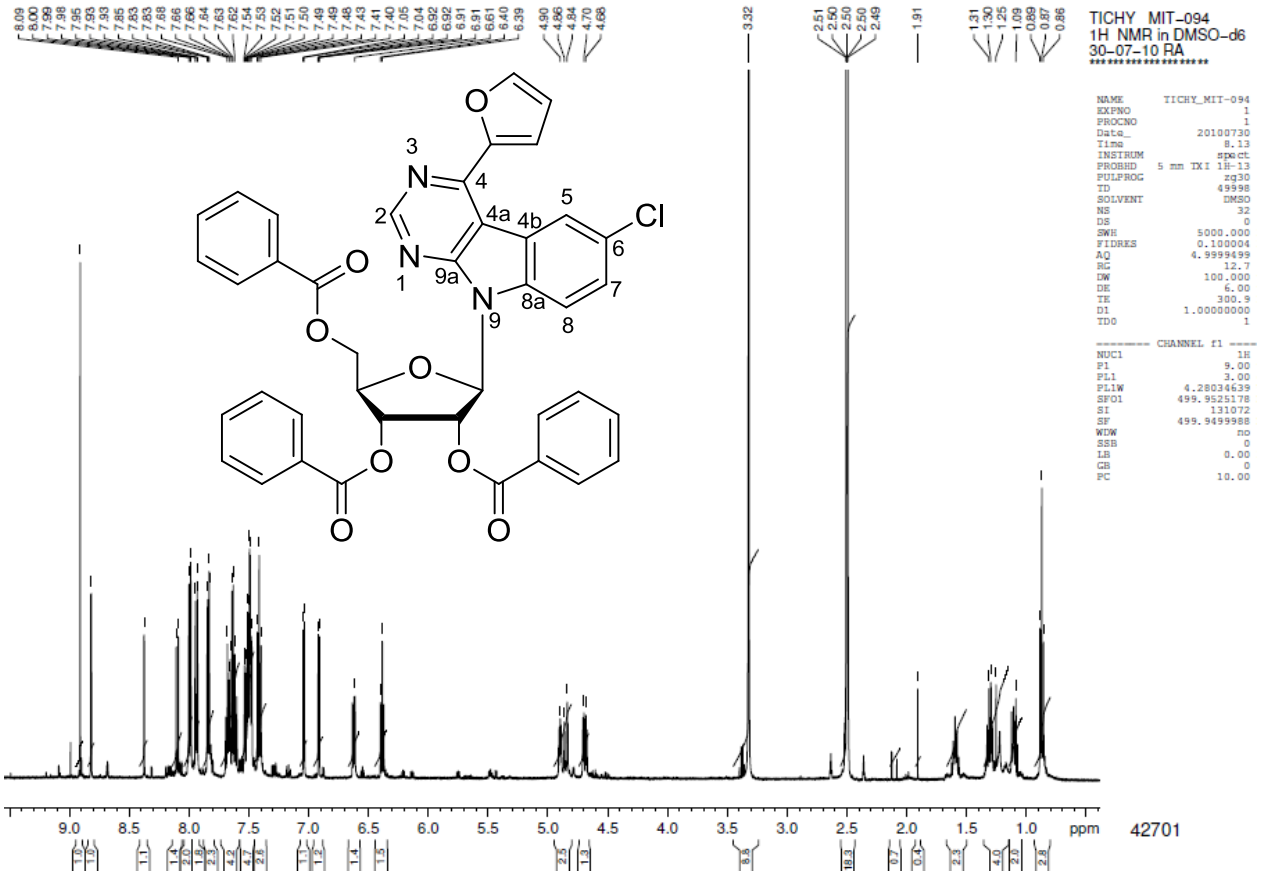
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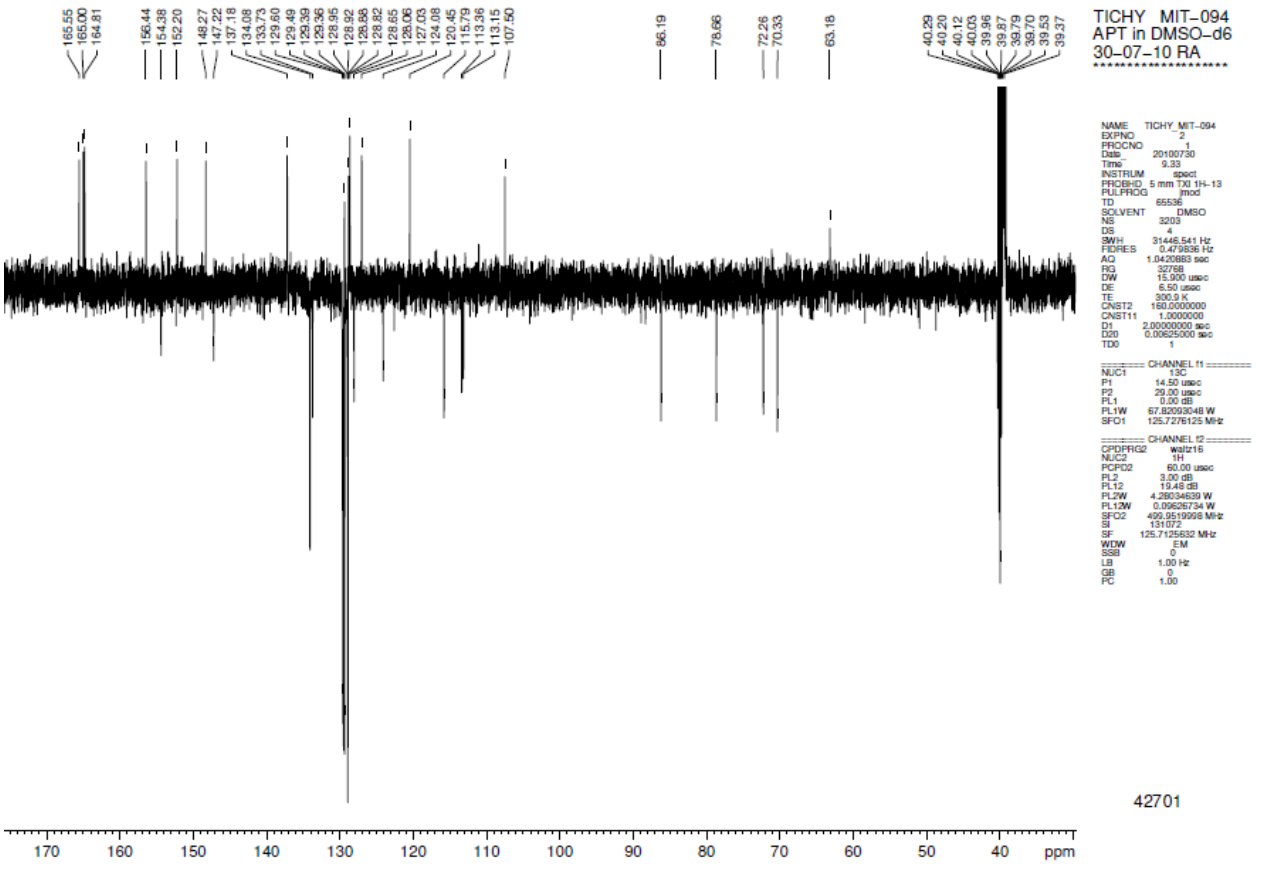
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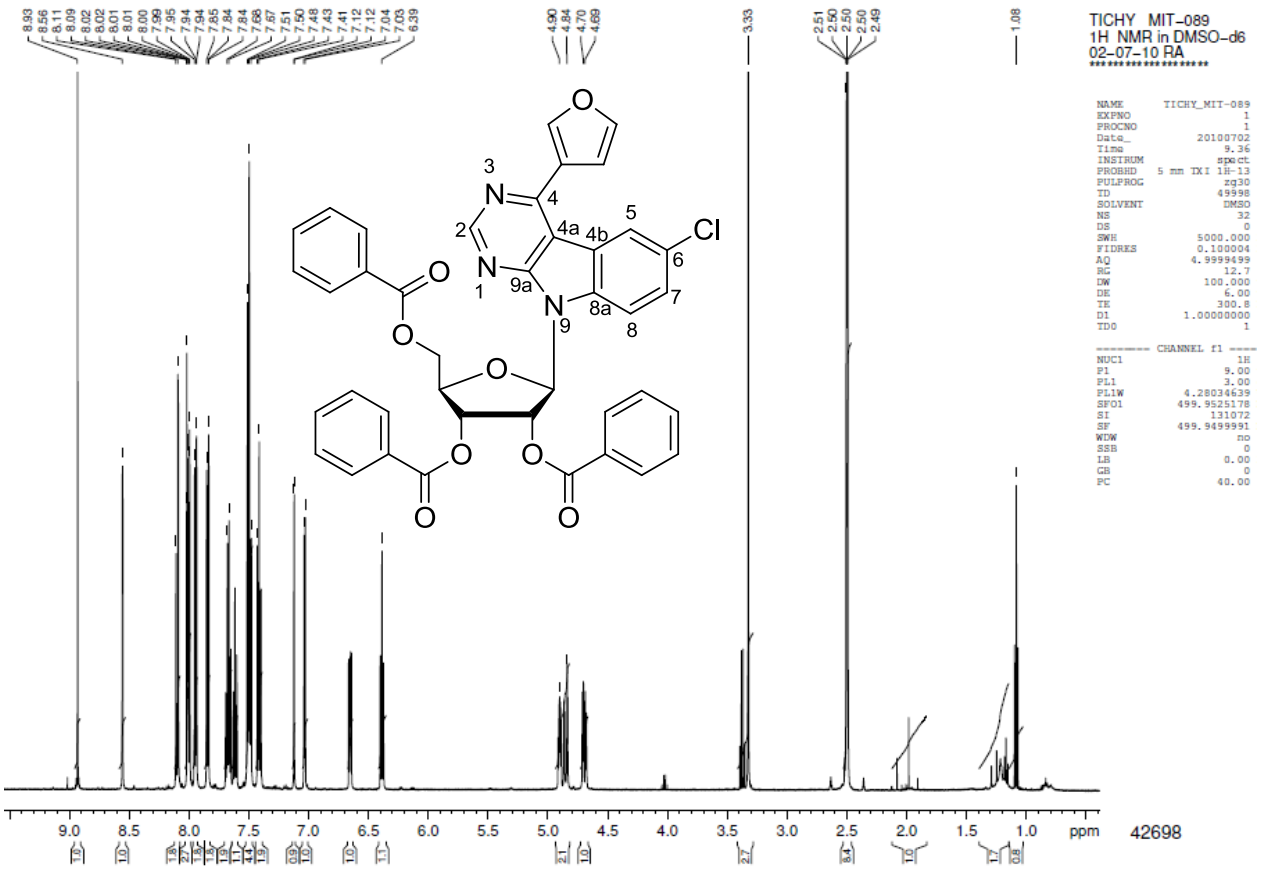
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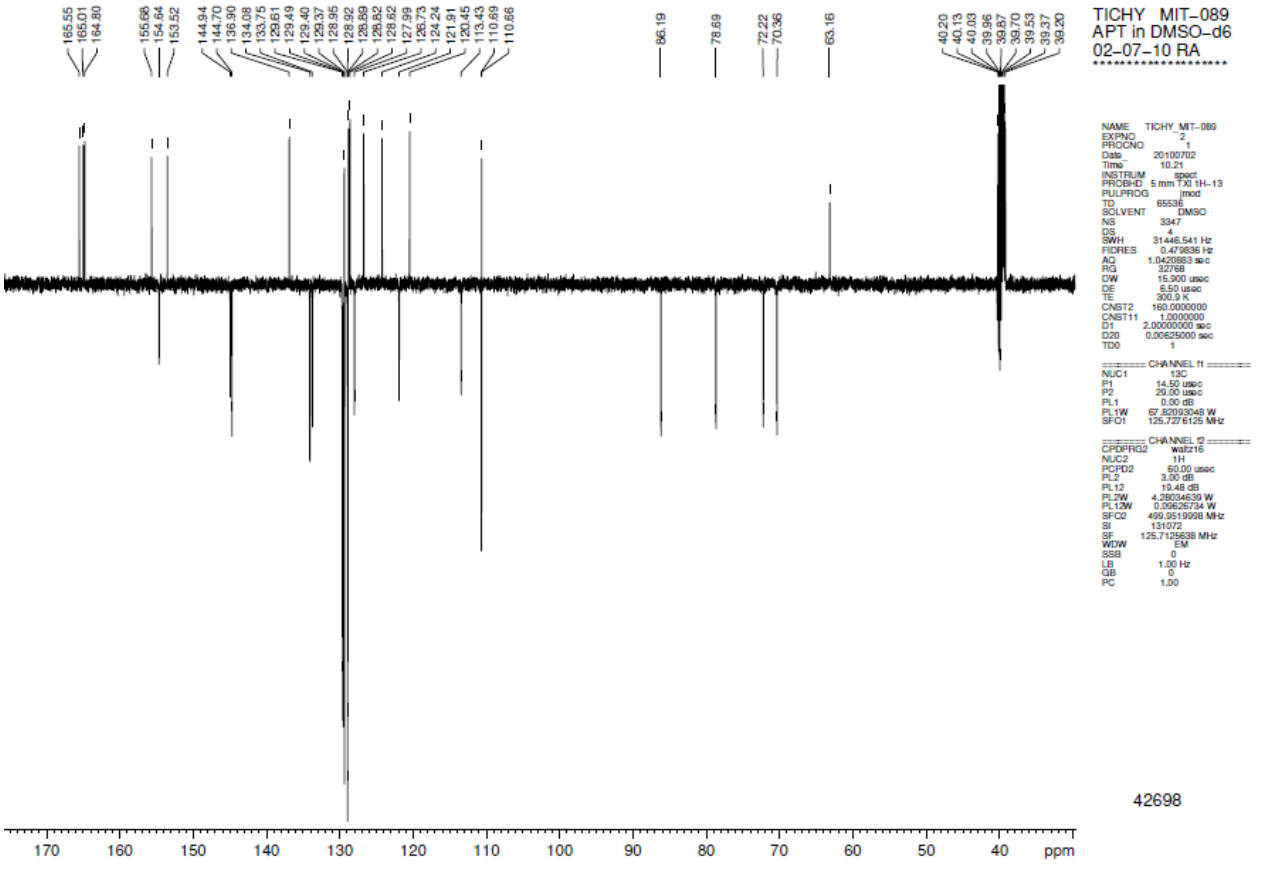
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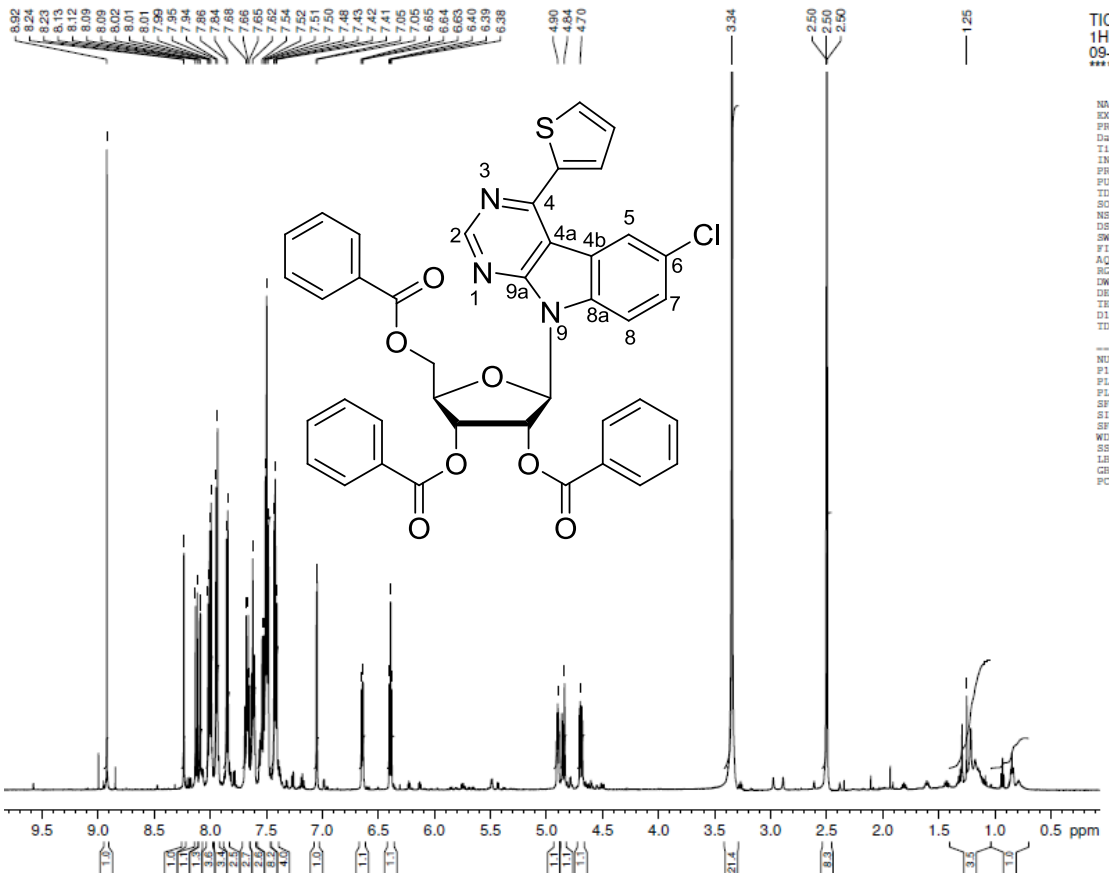
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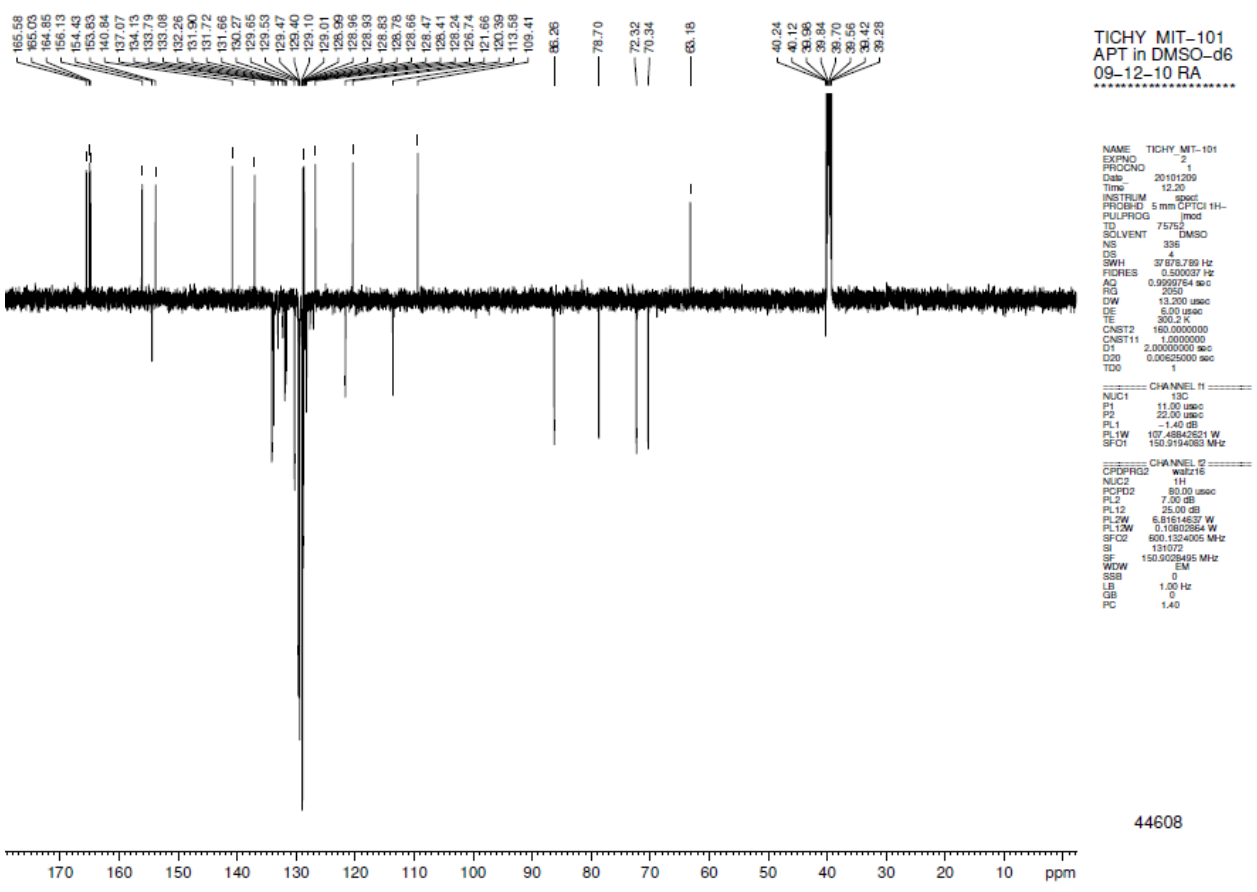
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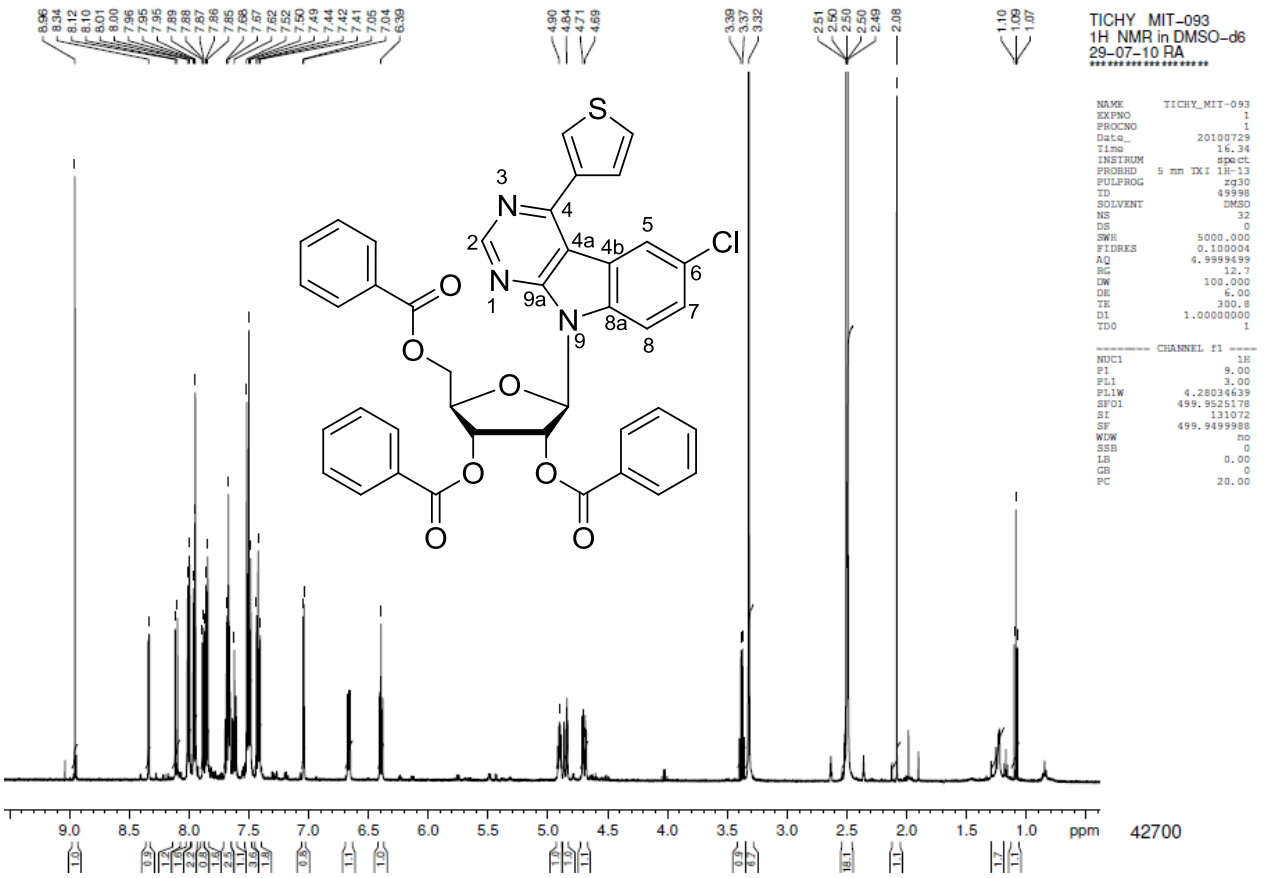
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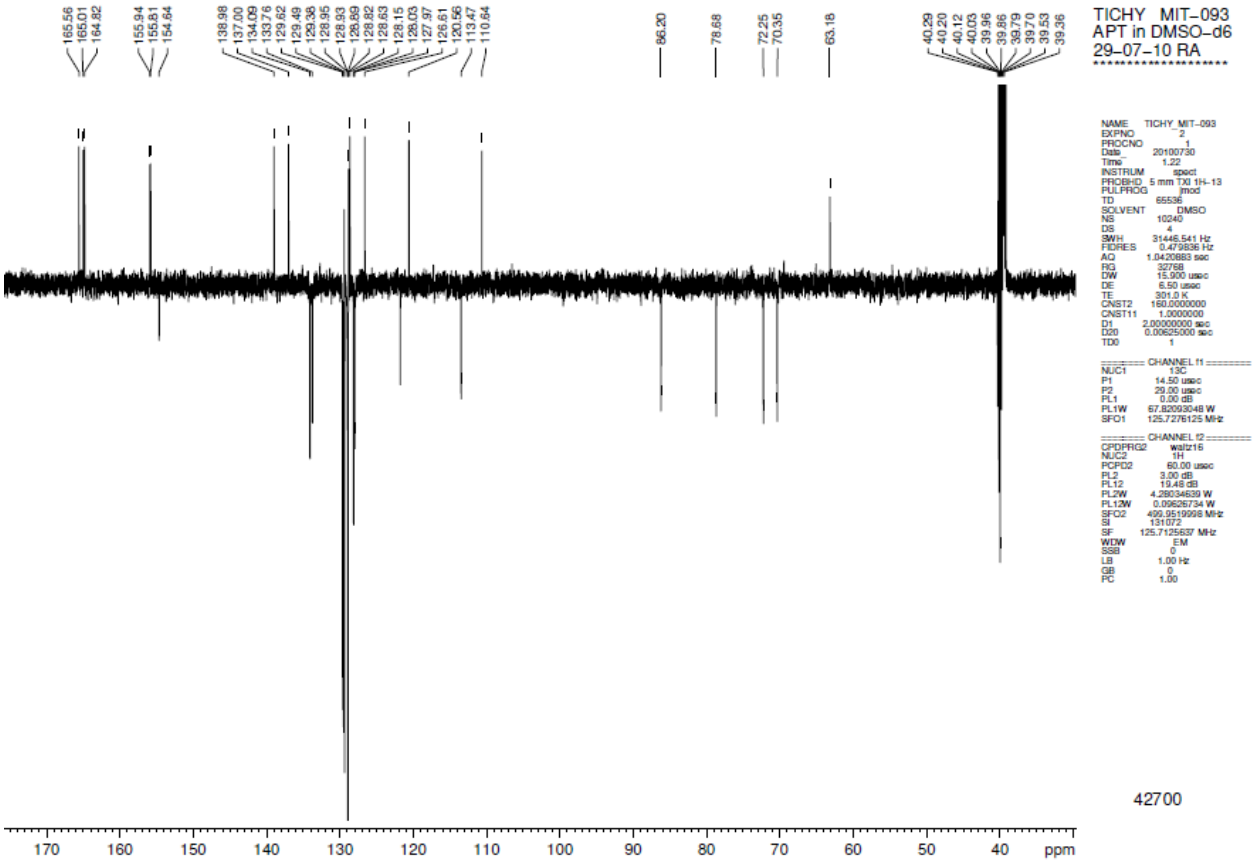
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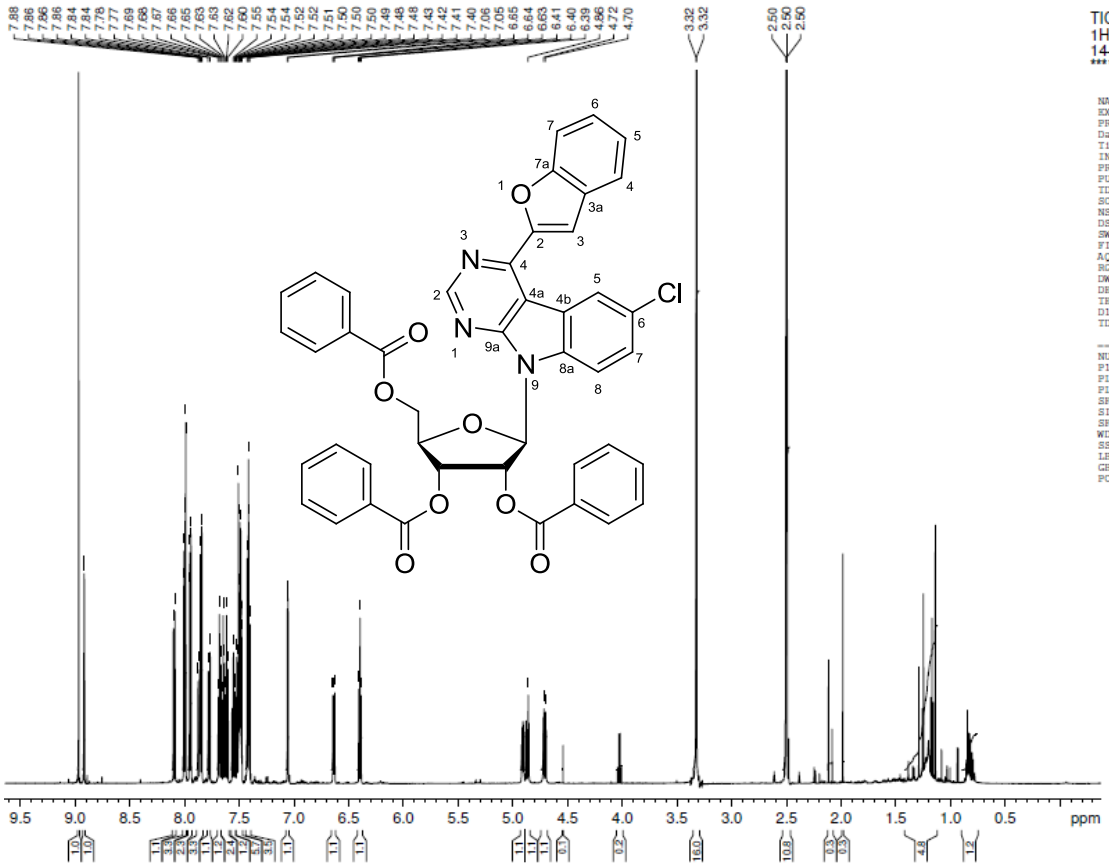
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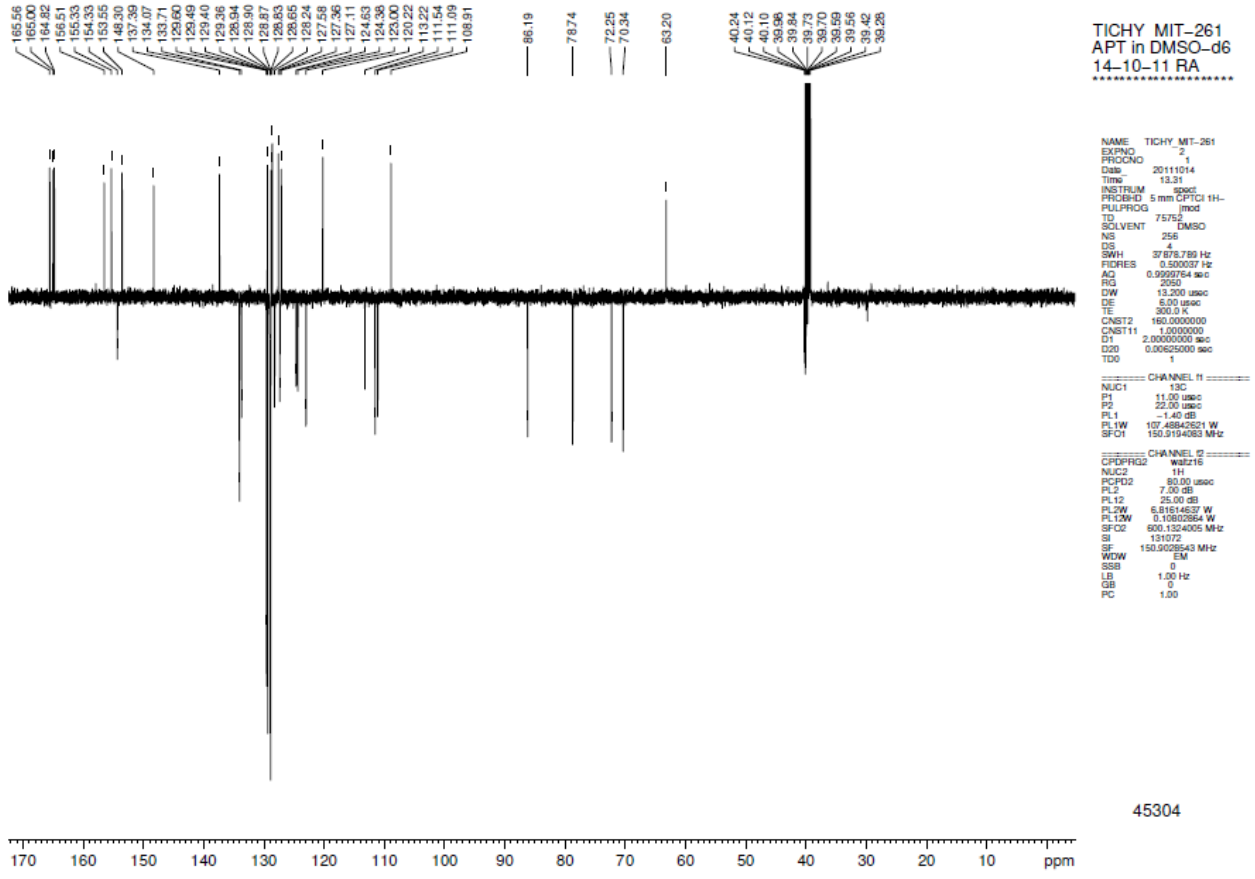
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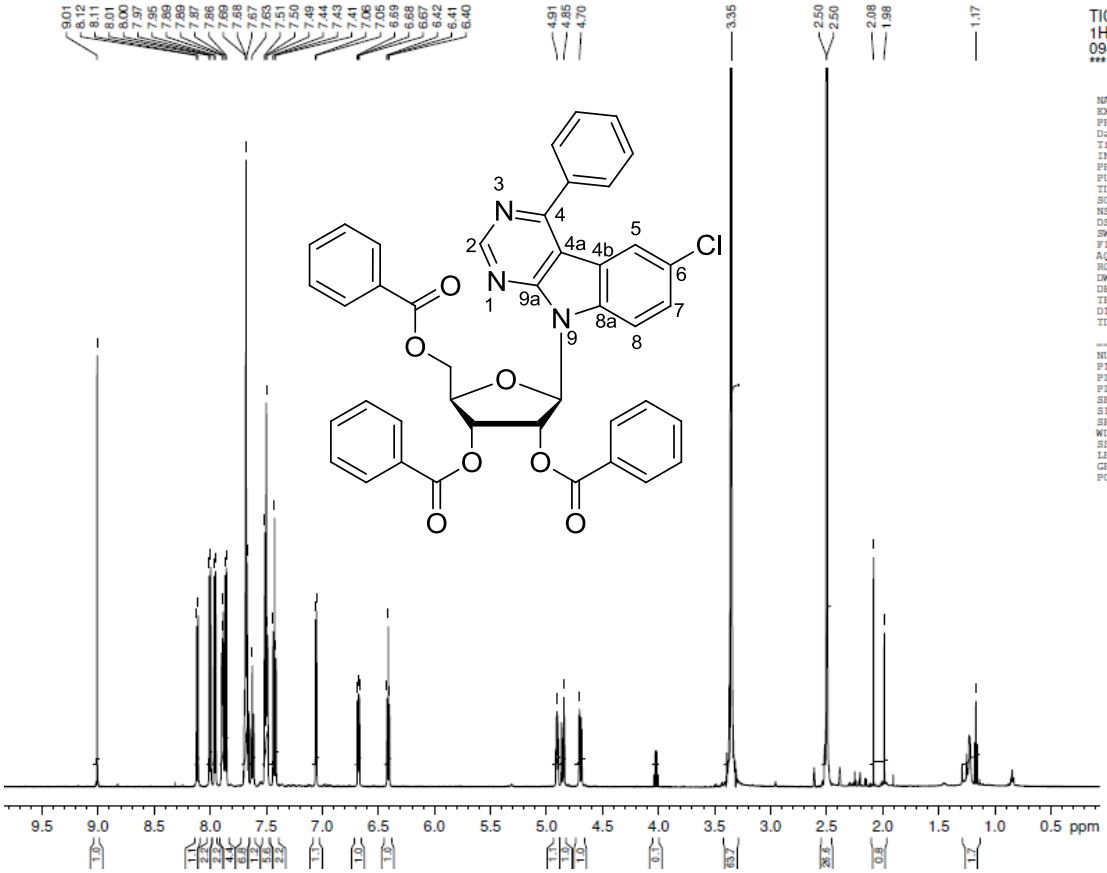
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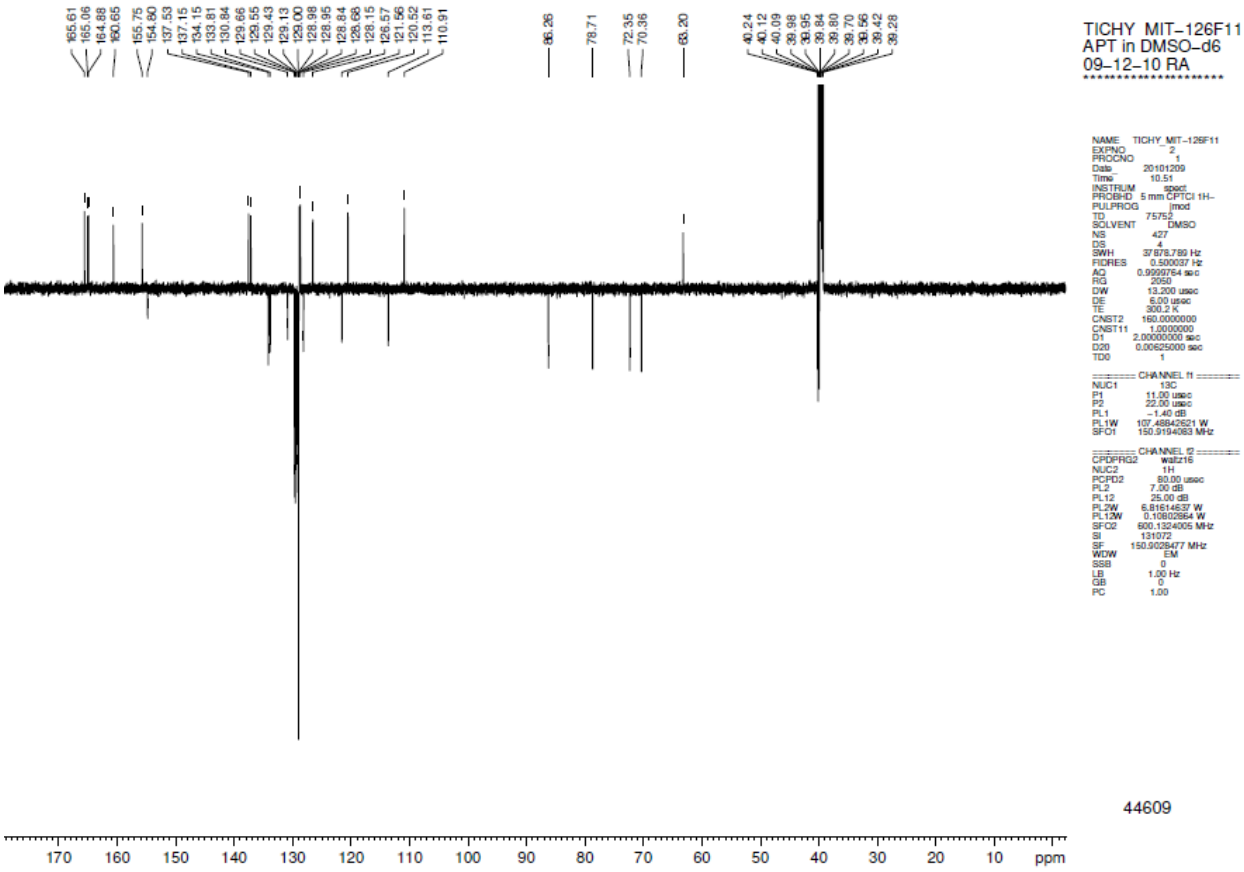
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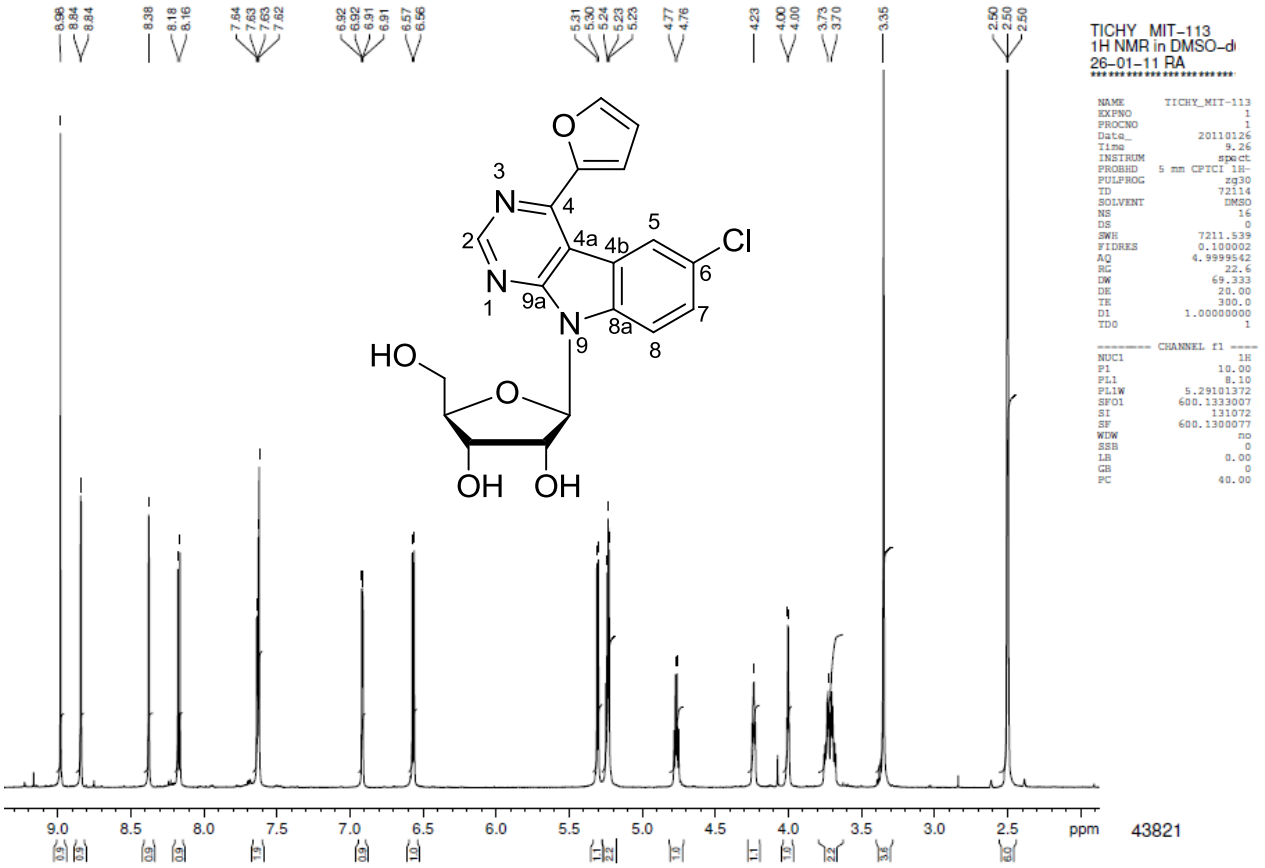
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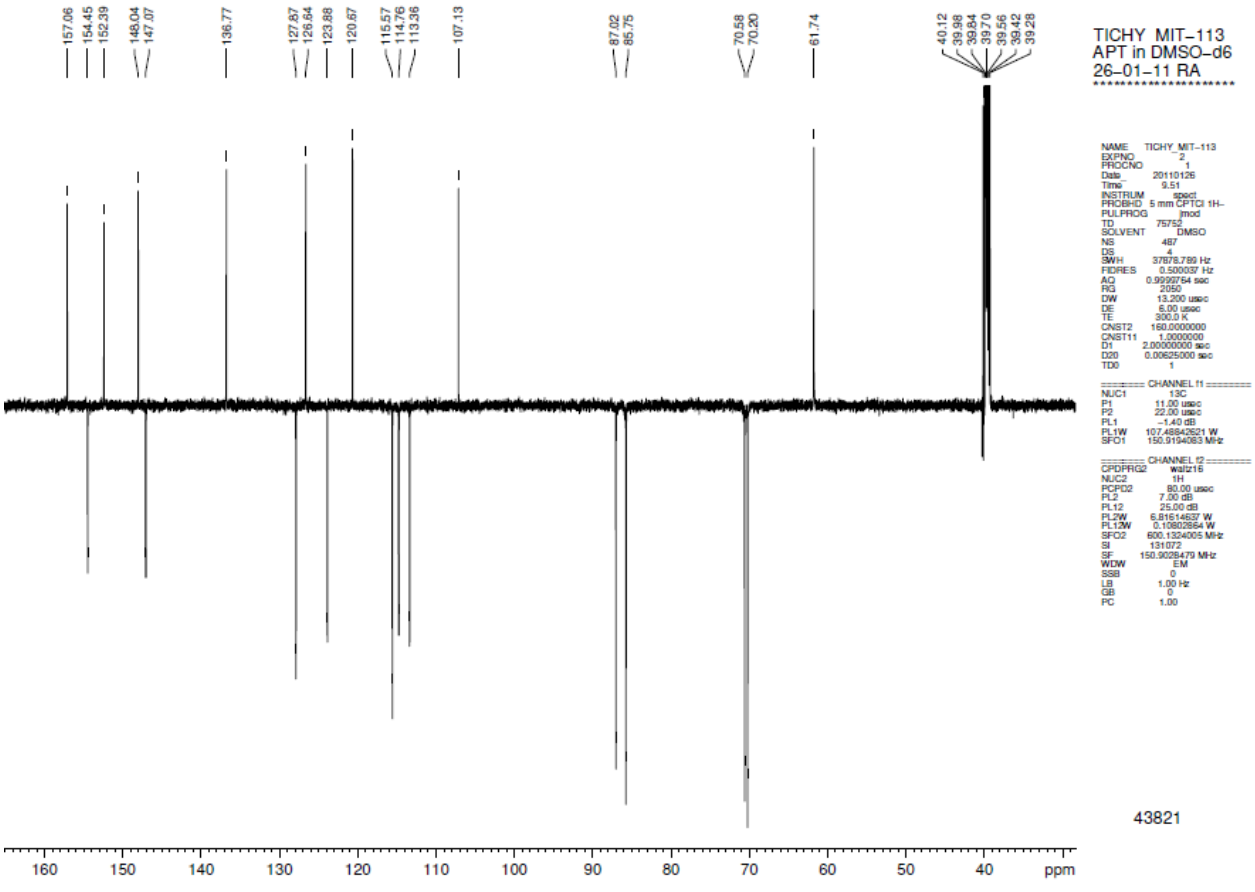
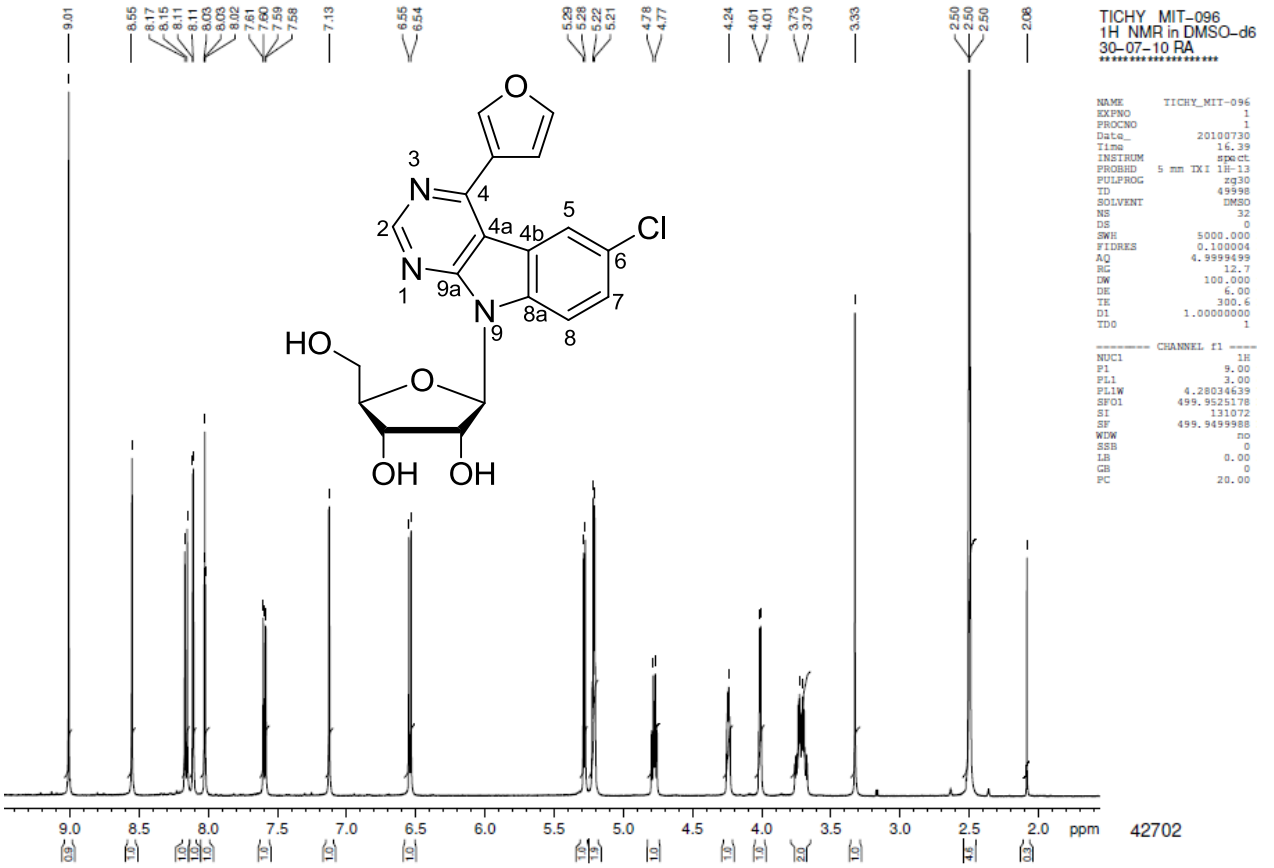
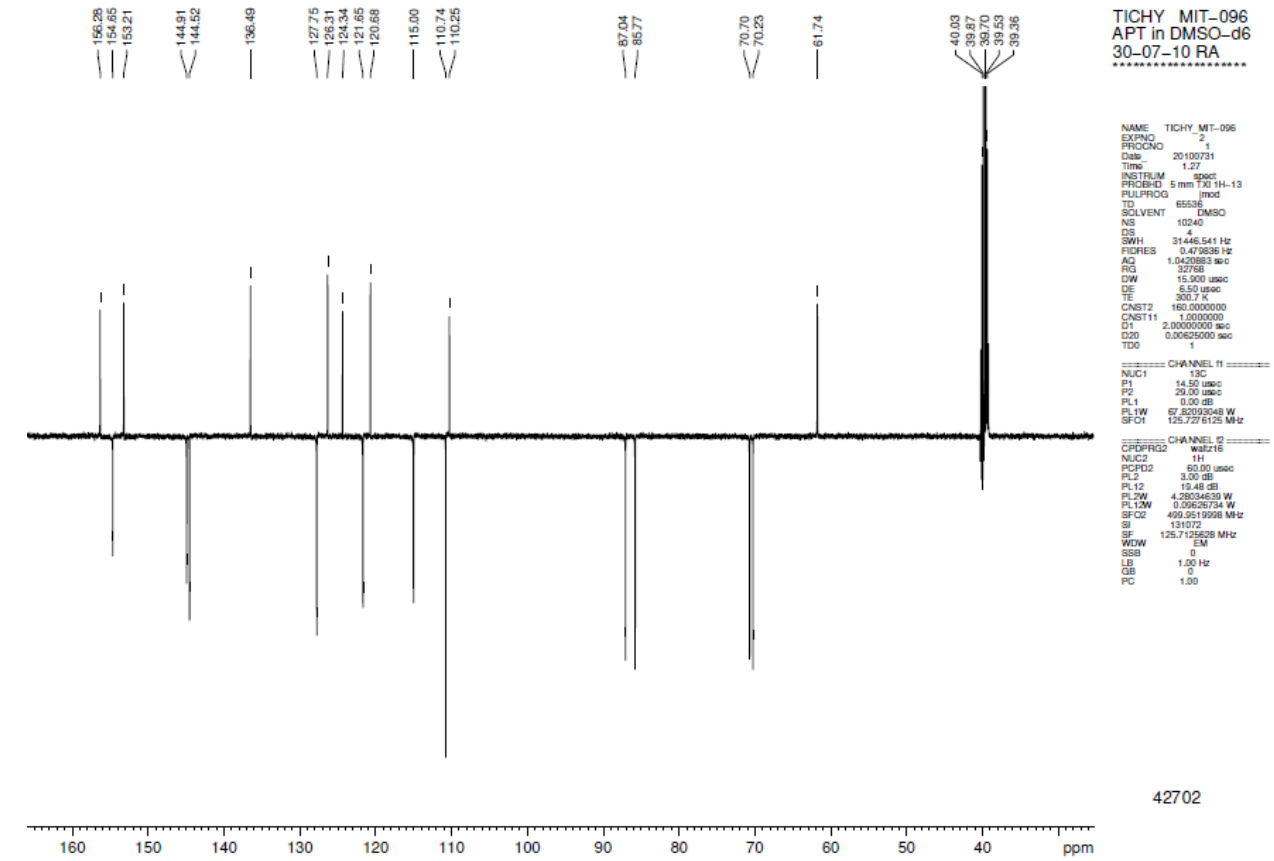
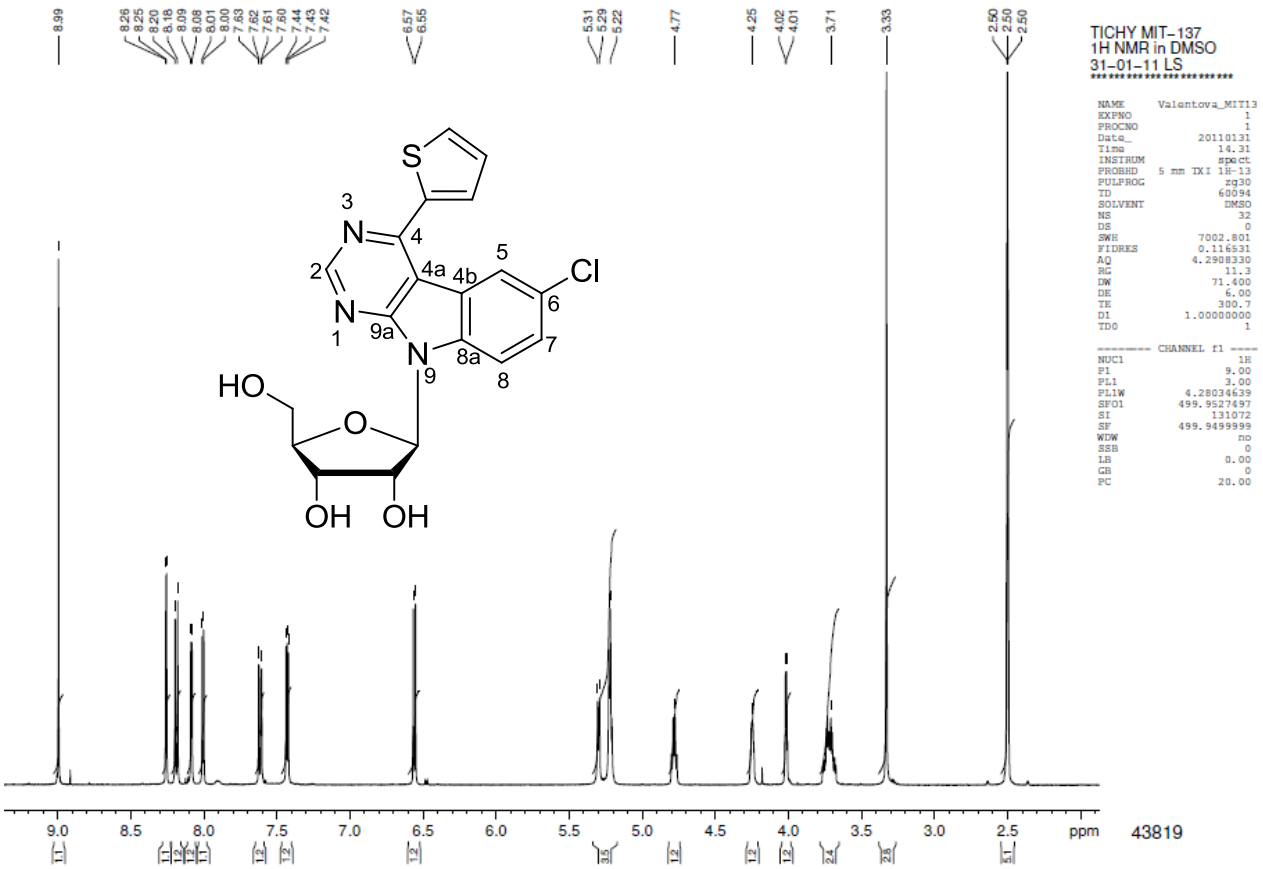

157.06
154.45
152.39
148.04
147.07
136.77
127.87
126.84
123.88
120.67
115.57
114.76
113.36
107.13
87.02
85.75
70.58
70.20
61.74
40.12
39.98
39.84
39.70
39.56
39.42
39.28
TICHY_MIT-113
APT in DMSO-d6
26-01-11 RA
NAME TICHY_MIT-113
EXPNO 2
PROCNO 1
Date_ 20110126
Time 9.51
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG jmod
TD 75752
SOLVENT DMSO
NS 487
DS 4
SWH 37878.789 Hz
FIDRES 0.500037 Hz
AQ 0.9999764 sec
RG 2050
DW 13.200 usec
DE 6.00 usec
TE 300.0 K
CNST2 160.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00625000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 -1.40 dB
PL1W 107.46842621 W
SFO1 150.9194083 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 7.00 dB
PL12 25.00 dB
PL2W 6.81614637 W
PL12W 0.10802864 W
SFO2 600.1324005 MHz
SI 131072
SF 150.9028479 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
ppm
43821

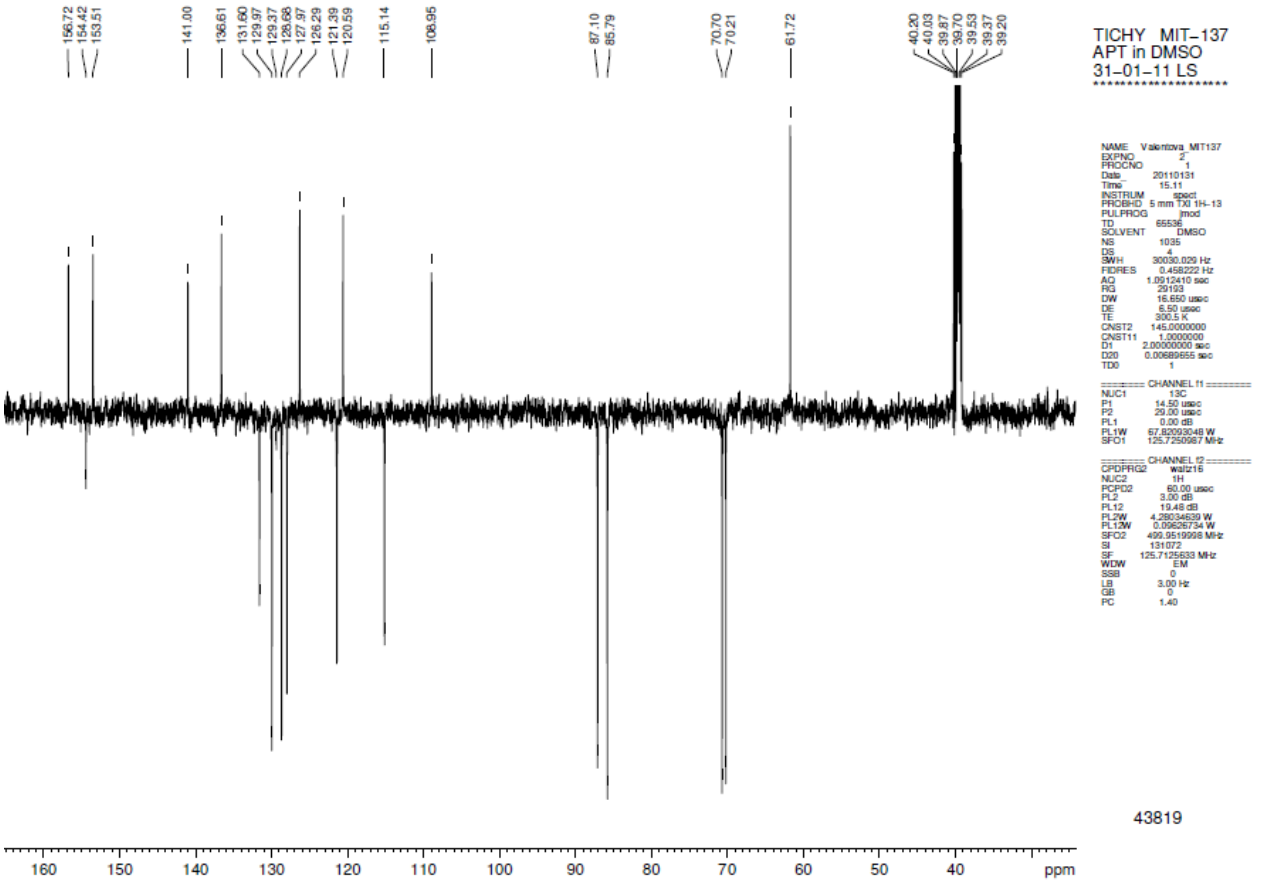
18b


TICHY_MIT-096
1H NMR in DMSO-d6
30-07-10 RA
42702

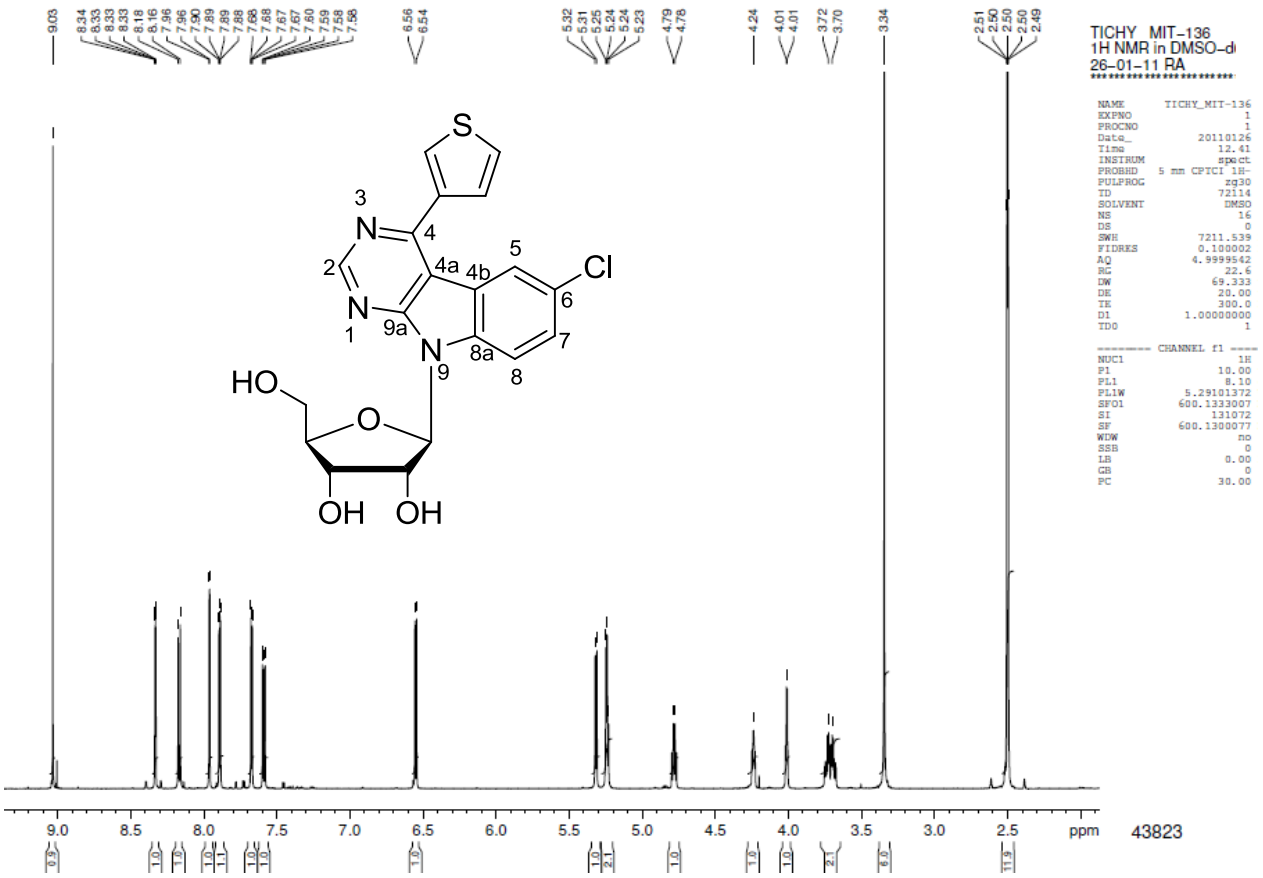

TICHY_MIT-096
APT in DMSO-d6
30-07-10 RA
42702

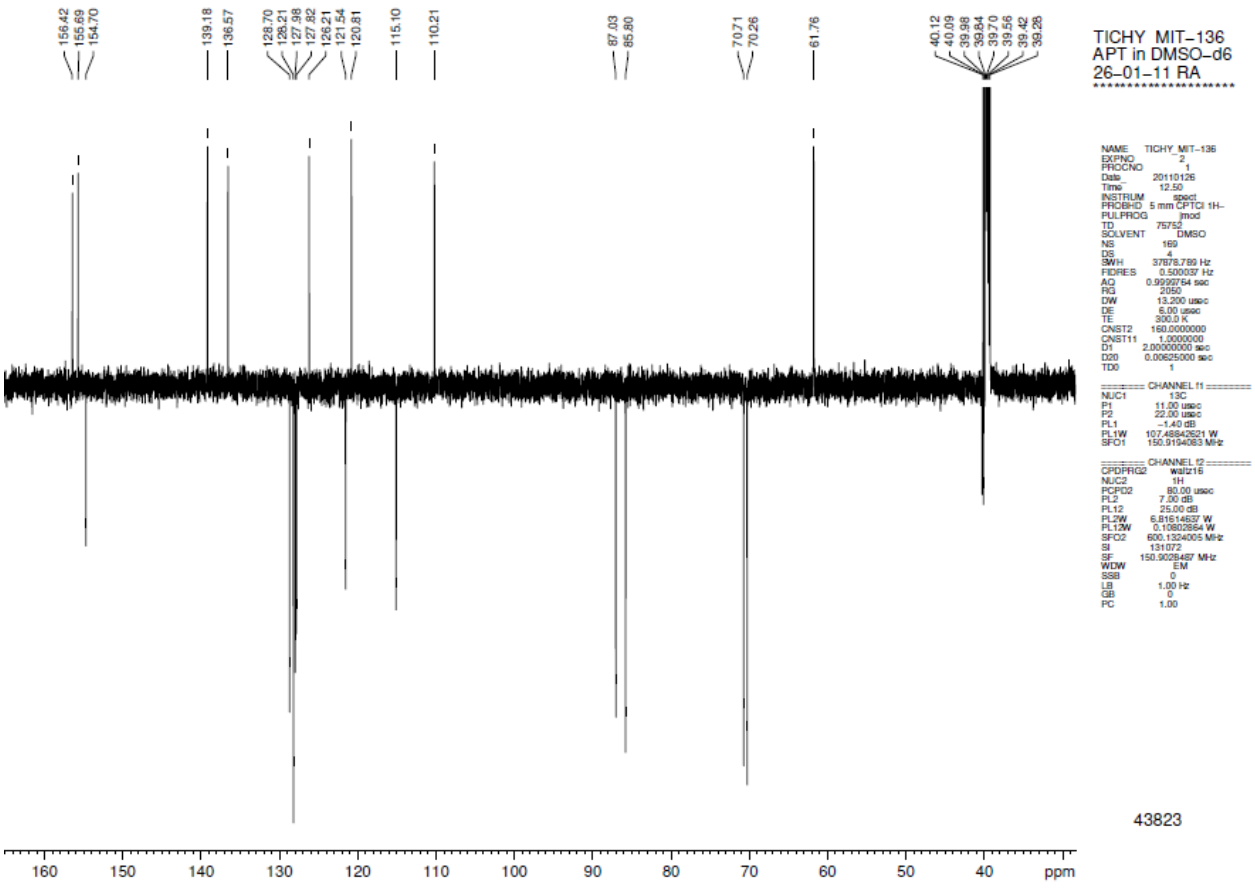
18c


8.99
8.28
8.25
8.20
8.18
8.09
8.08
8.01
8.00
7.63
7.62
7.61
7.60
7.44
7.43
7.42
6.57
6.55
5.31
5.29
5.22
4.77
4.25
4.02
4.01
3.71
3.33
2.50
2.50
2.50
S
N
N
N
Cl
HO
O
OH
OH
TICHY MIT-137
1H NMR in DMSO
31-01-11 LS
NAME Valentova_MIT13
EXPNO 1
PROCNO 1
Date_ 20110131
Time 14.31
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG zg30
TD 60094
SOLVENT DMSO
NS 32
DS 0
SWH 7002.801
FIDRES 0.116531
AQ 4.2908330
RG 11.3
DW 71.400
DE 6.00
TE 300.7
D1 1.00000000
TD0 1
CHANNEL f1
NUC1 1H
P1 9.00
PL1 3.00
PL1W 4.28034639
SFO1 499.9527497
SI 131072
SF 499.9499999
WDW no
SSB 0
LB 0.00
GB 0
PC 20.00
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
ppm
43819

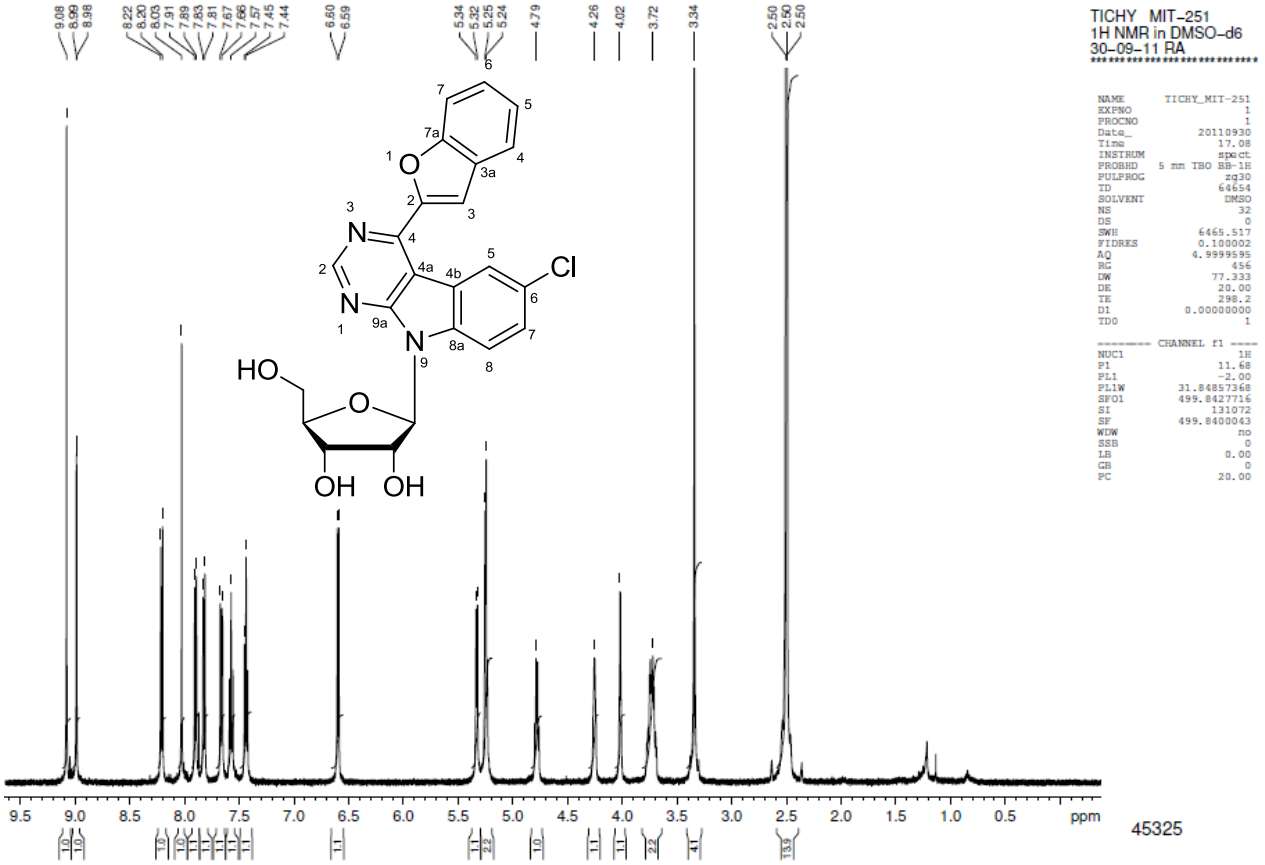

156.72
154.42
153.51
141.00
136.61
131.60
129.97
129.37
128.66
127.97
126.29
121.39
120.59
115.14
108.95
87.10
85.79
70.70
70.21
61.72
40.20
40.03
39.87
39.70
39.53
39.37
39.20
TICHY MIT-137
APT in DMSO
31-01-11 LS
NAME Valentova_MIT137
EXPNO 2
PROCNO 1
Date_ 20110131
Time 15.11
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 1035
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 29193
DW 16.650 usec
DE 6.50 usec
TE 300.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 14.50 usec
P2 29.00 usec
PL1 0.00 dB
PL1W 67.82093048 W
SFO1 125.7250987 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 3.00 dB
PL12 19.46 dB
PL2W 4.28034639 W
PL12W 0.09626734 W
SFO2 499.9519998 MHz
SI 131072
SF 125.7125633 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm
43819

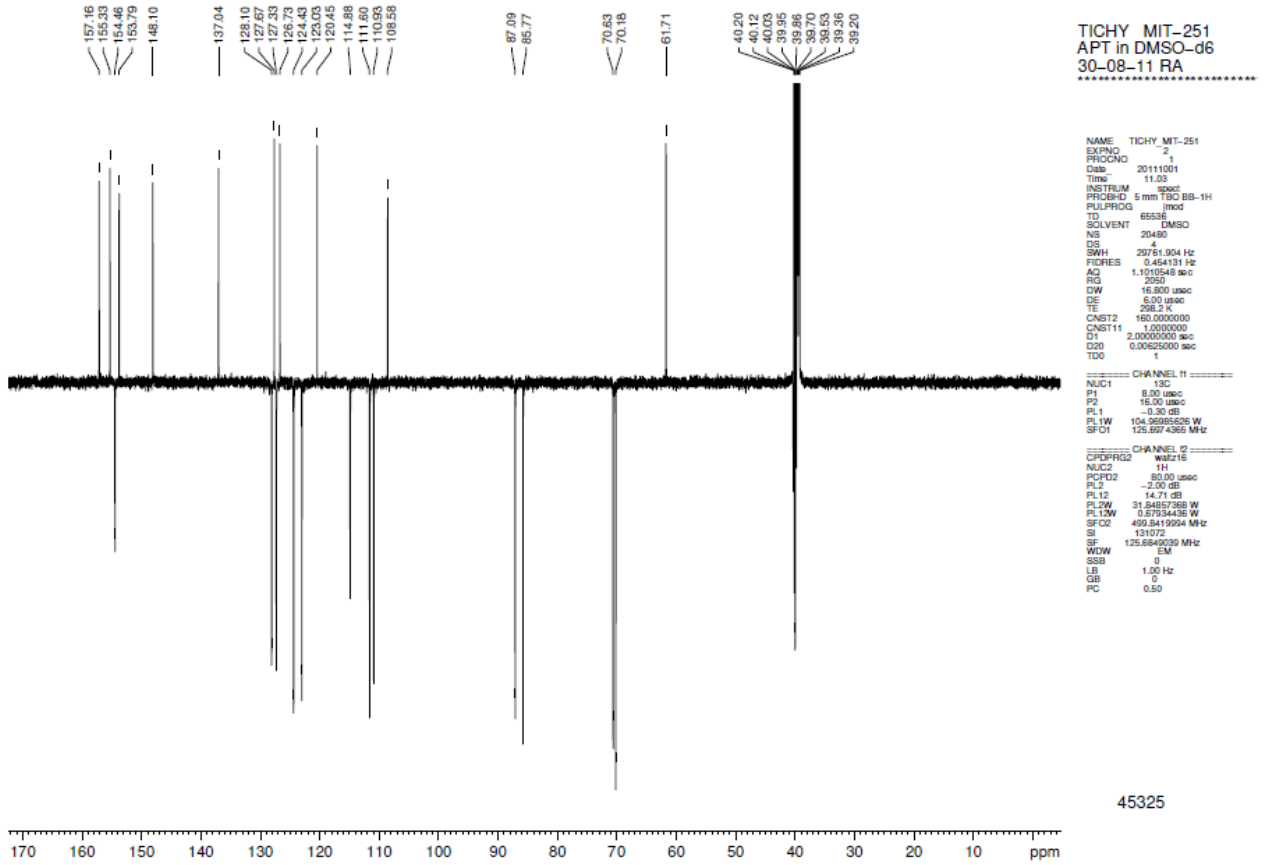
18d


9.03
8.34 8.33 8.33 8.33 8.18 8.16 7.96 7.96 7.90 7.89 7.89 7.88 7.66 7.68 7.67 7.67 7.60 7.59 7.58 7.56
6.56 6.54
5.32 5.31 5.25 5.24 5.24 5.23
4.79 4.78
4.24
4.01 4.01
3.72 3.70
3.34
2.51 2.50 2.50 2.50 2.49
S
N
N
N
Cl
HO
O
OH
OH
TICHY_MIT-136
1H NMR in DMSO-d
26-01-11 RA
NAME TICHY_MIT-136
EXPNO 1
PROCNO 1
Date_ 20110126
Time 12.41
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 72114
SOLVENT DMSO
NS 16
DS 0
SWH 7211.539
FIDRES 0.100002
AQ 4.9999542
RG 22.6
DW 69.333
DE 20.00
TE 300.0
D1 1.00000000
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00
PL1 8.10
PL1W 5.29101372
SFO1 600.1333007
SI 131072
SF 600.1300077
WDW no
SSB 0
LB 0.00
GB 0
PC 30.00
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 ppm
43823

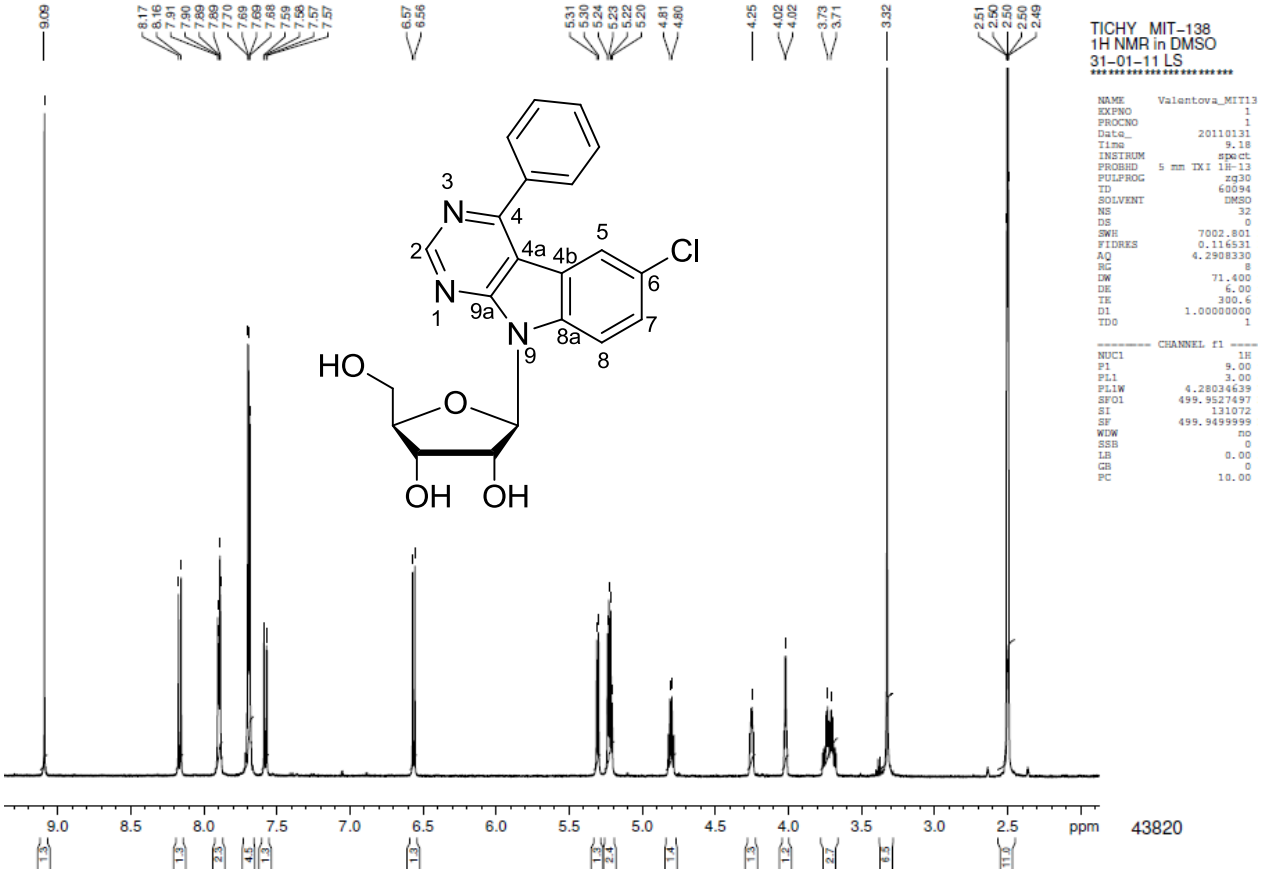

156.42
155.69
154.70
139.18
136.57
128.70
128.21
127.98
127.82
126.21
121.54
120.81
115.10
110.21
87.03
85.80
70.71
70.26
61.76
40.12
40.09
39.98
39.84
39.70
39.56
39.42
39.28
TICHY_MIT-136
APT in DMSO-d6
26-01-11 RA
NAME TICHY_MIT-136
EXPNO 2
PROCNO 1
Date_ 20110126
Time 12.50
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG jmod
TD 75752
SOLVENT DMSO
NS 169
DS 4
SWH 37878.789 Hz
FIDRES 0.500037 Hz
AQ 0.9999764 sec
RG 2050
DW 13.200 usec
DE 6.00 usec
TE 300.0 K
CNST2 160.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00625000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 -1.40 dB
PL1W 107.48842621 W
SFO1 150.9194083 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 7.00 dB
PL12 25.00 dB
PL2W 6.81614637 W
PL12W 0.10802864 W
SFO2 600.1324005 MHz
SI 131072
SF 150.9029487 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
160 150 140 130 120 110 100 90 80 70 60 50 40 ppm
43823

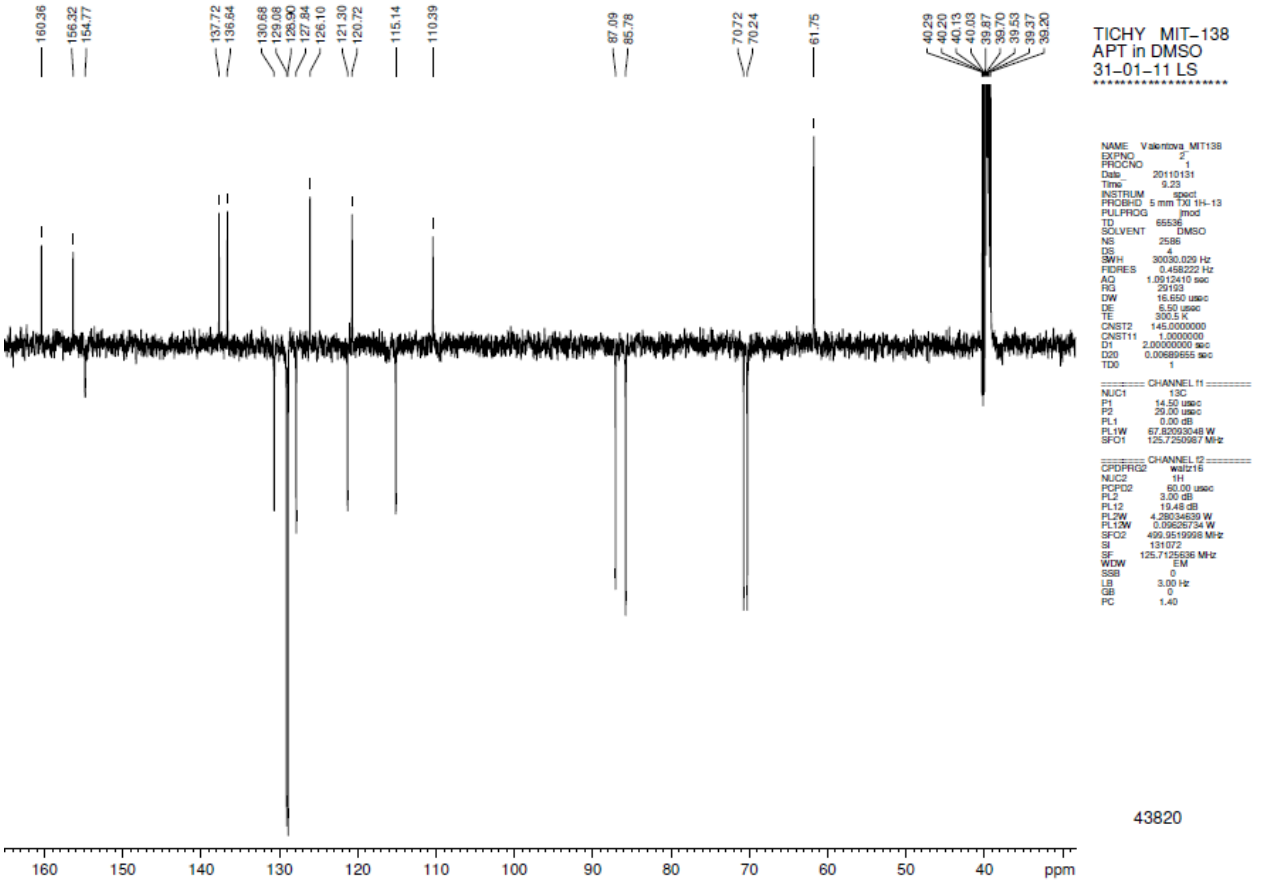
18e


9.08
8.99
8.98
8.22
8.20
8.03
7.91
7.89
7.83
7.81
7.67
7.66
7.57
7.45
7.44
6.60
6.59
5.34
5.32
5.25
5.24
4.79
4.26
4.02
3.72
3.34
2.50
2.50
2.50
HO
OH
OH
Cl
TICHY_MIT-251
1H NMR in DMSO-d6
30-09-11 RA
45325
ppm

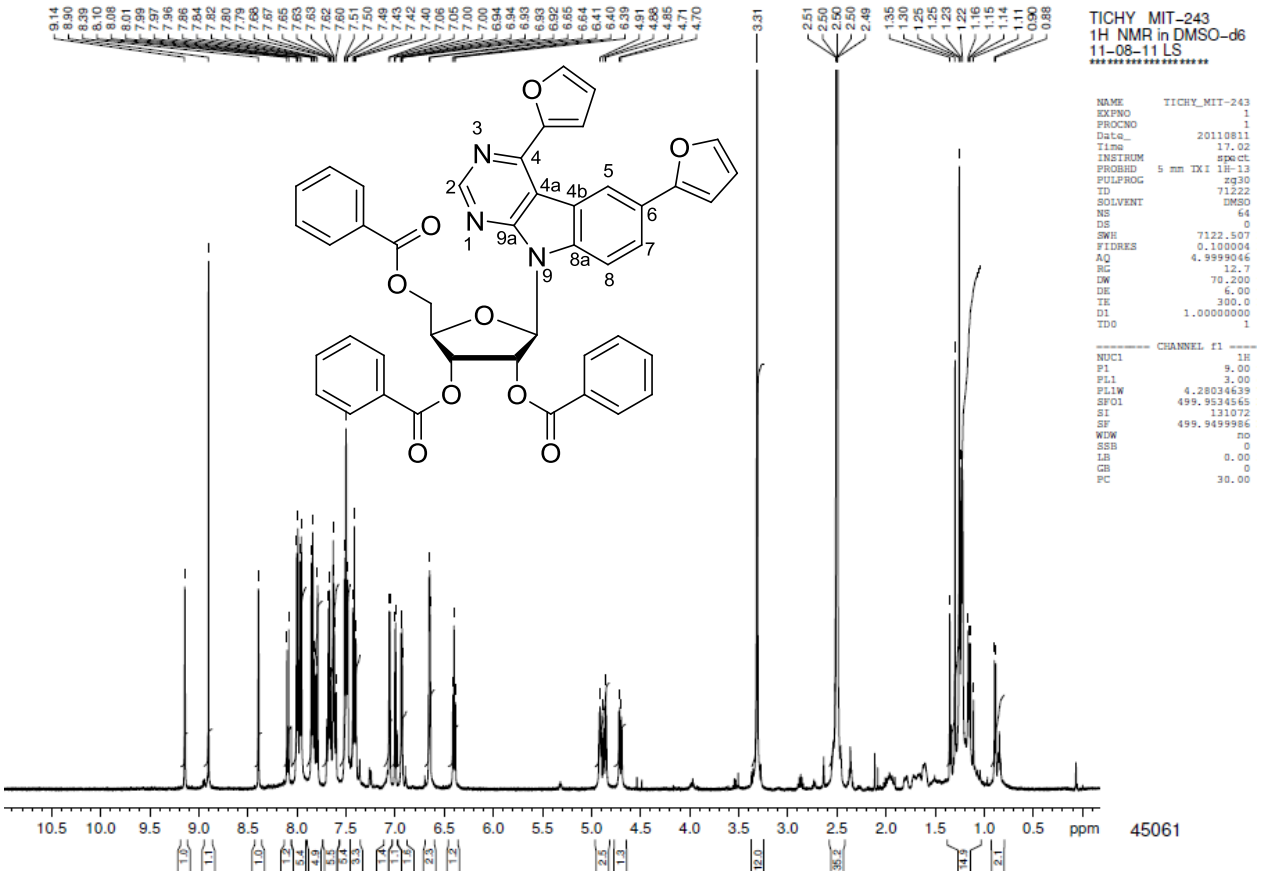

157.16
155.33
154.46
153.79
148.10
137.04
128.10
127.67
127.33
126.73
124.43
123.03
120.45
114.88
111.60
110.93
108.58
87.09
85.77
70.63
70.18
61.71
40.20
40.12
40.03
39.95
39.86
39.70
39.53
39.36
39.20
TICHY_MIT-251
APT in DMSO-d6
30-08-11 RA
45325
ppm

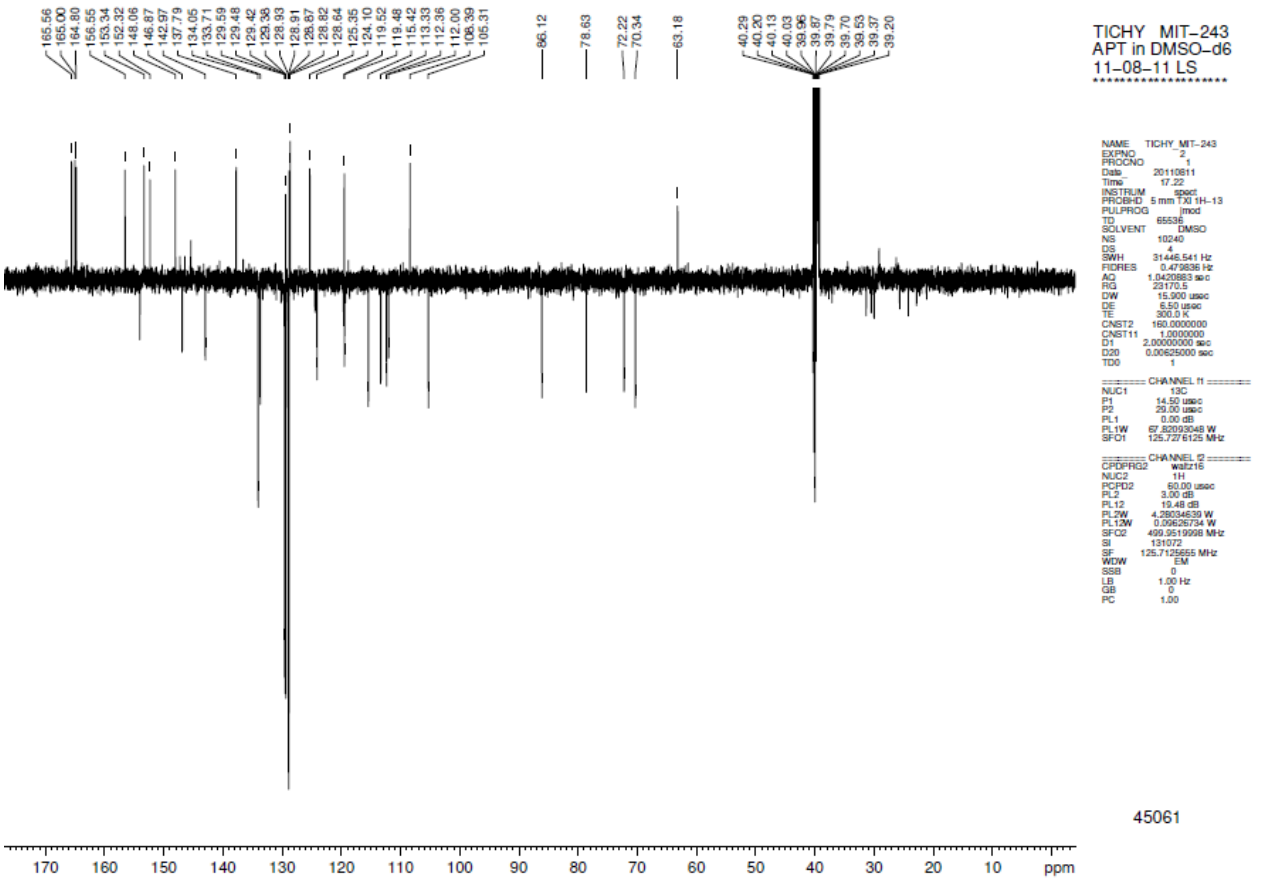
18f


TICHY MIT-138
1H NMR in DMSO
31-01-11 LS
43820
ppm

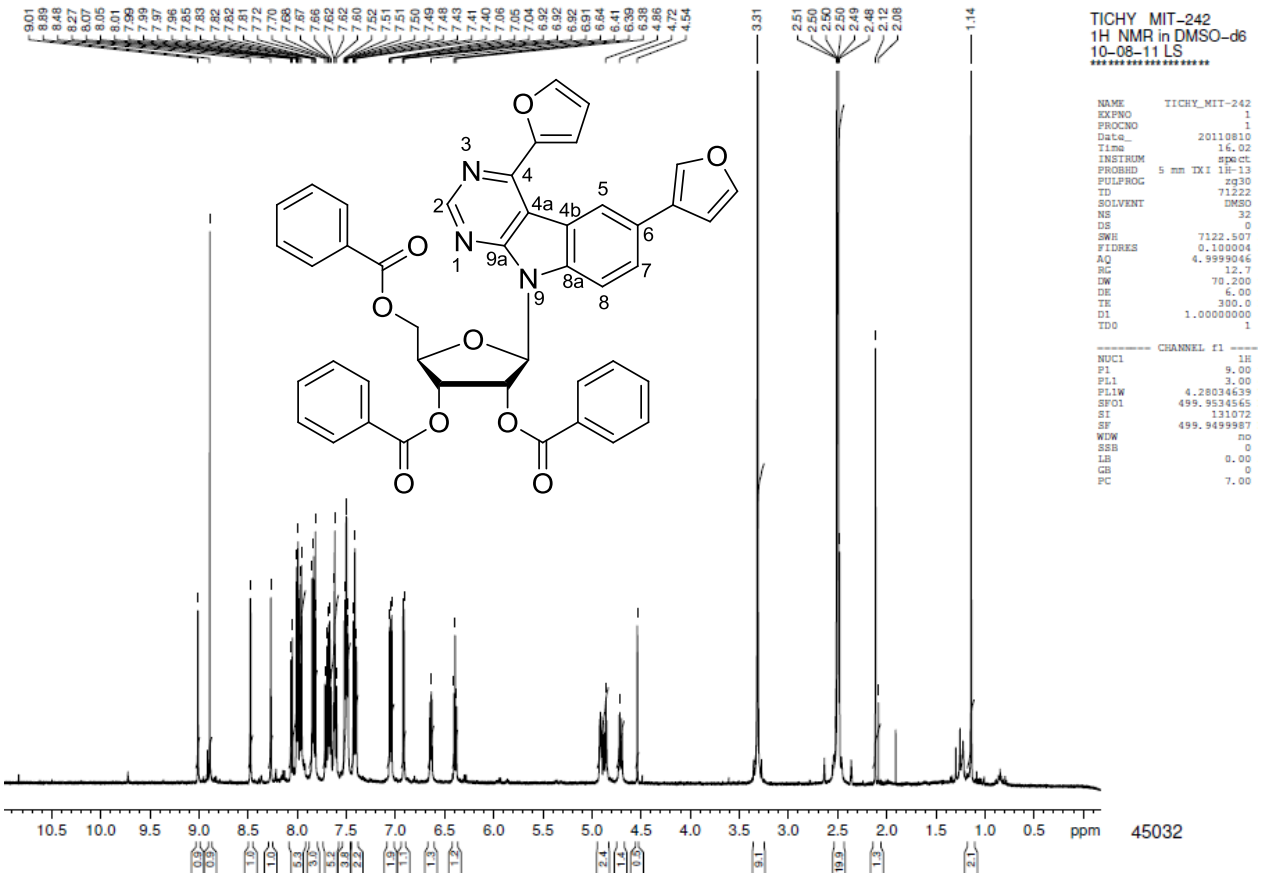

TICHY MIT-138
APT in DMSO
31-01-11 LS
43820
ppm

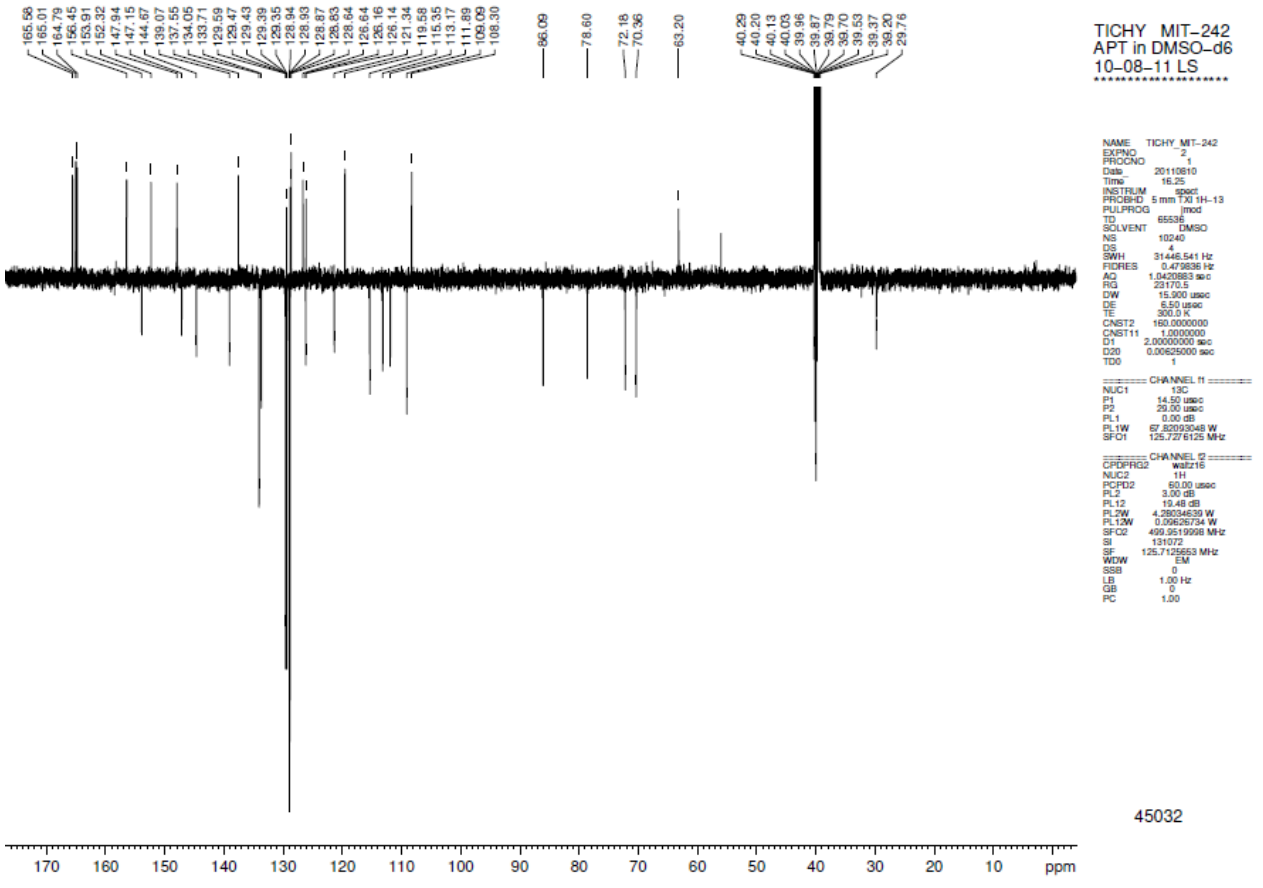
20a


TICHY MIT-243
1H NMR in DMSO-d6
11-08-11 LS
45061

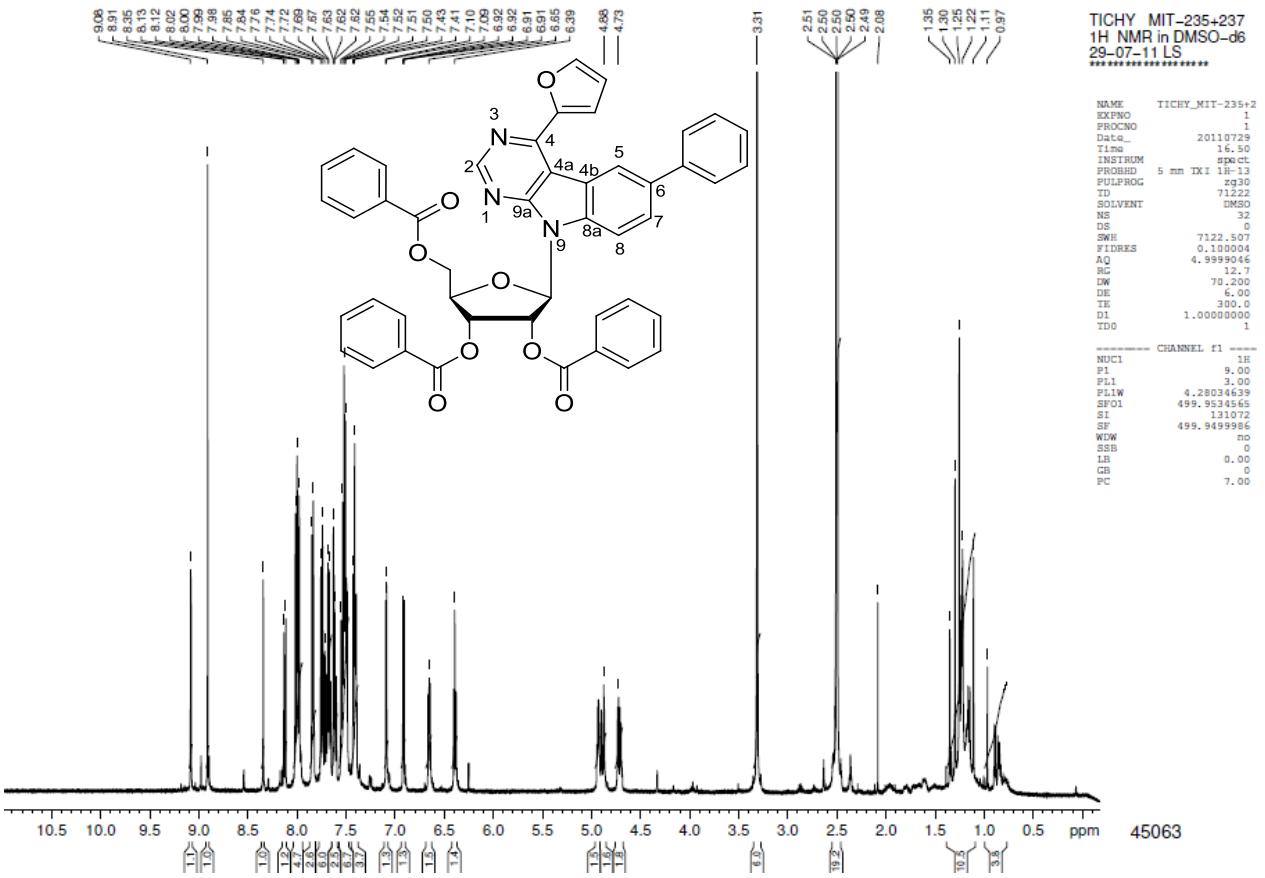

TICHY MIT-243
APT in DMSO-d6
11-08-11 LS
45061

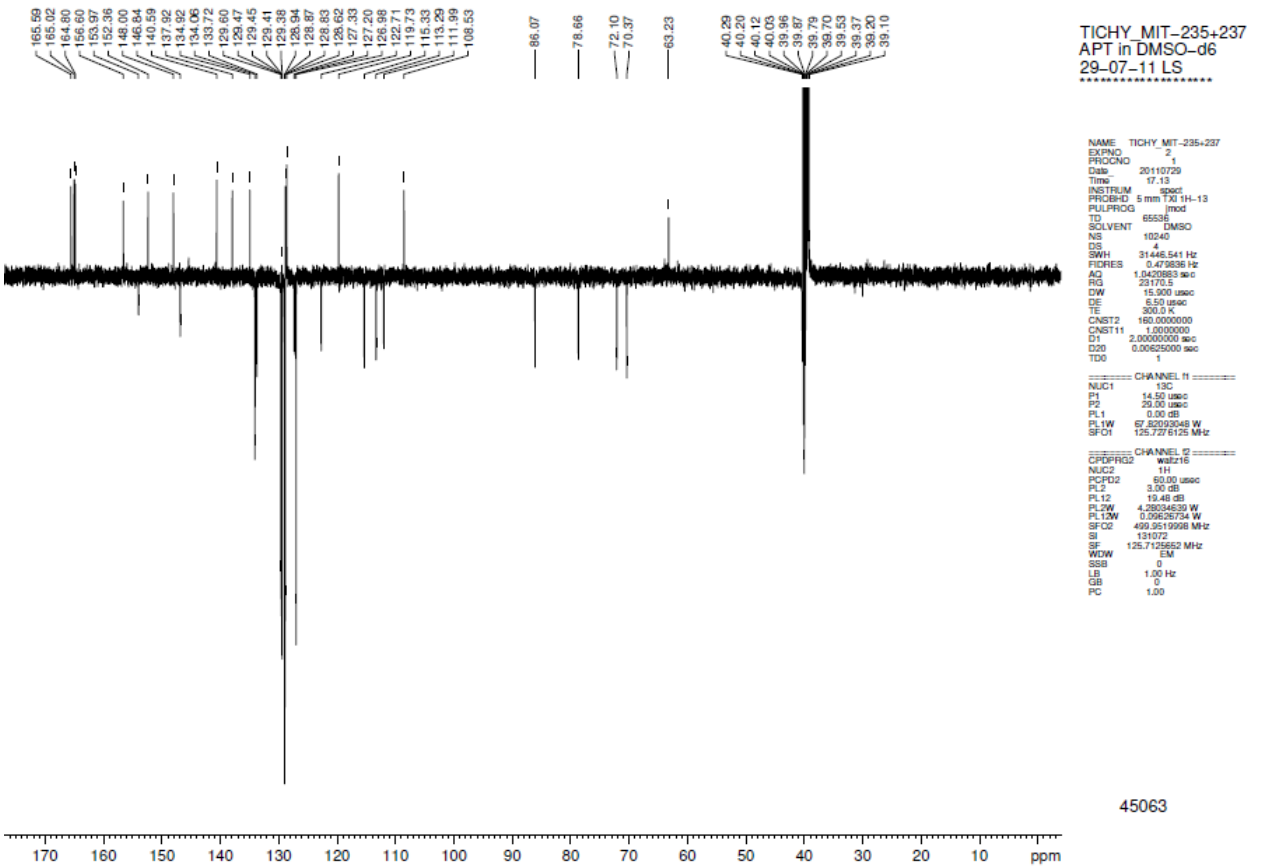
20b


TICHY MIT-242
1H NMR in DMSO-d6
10-08-11 LS
45032

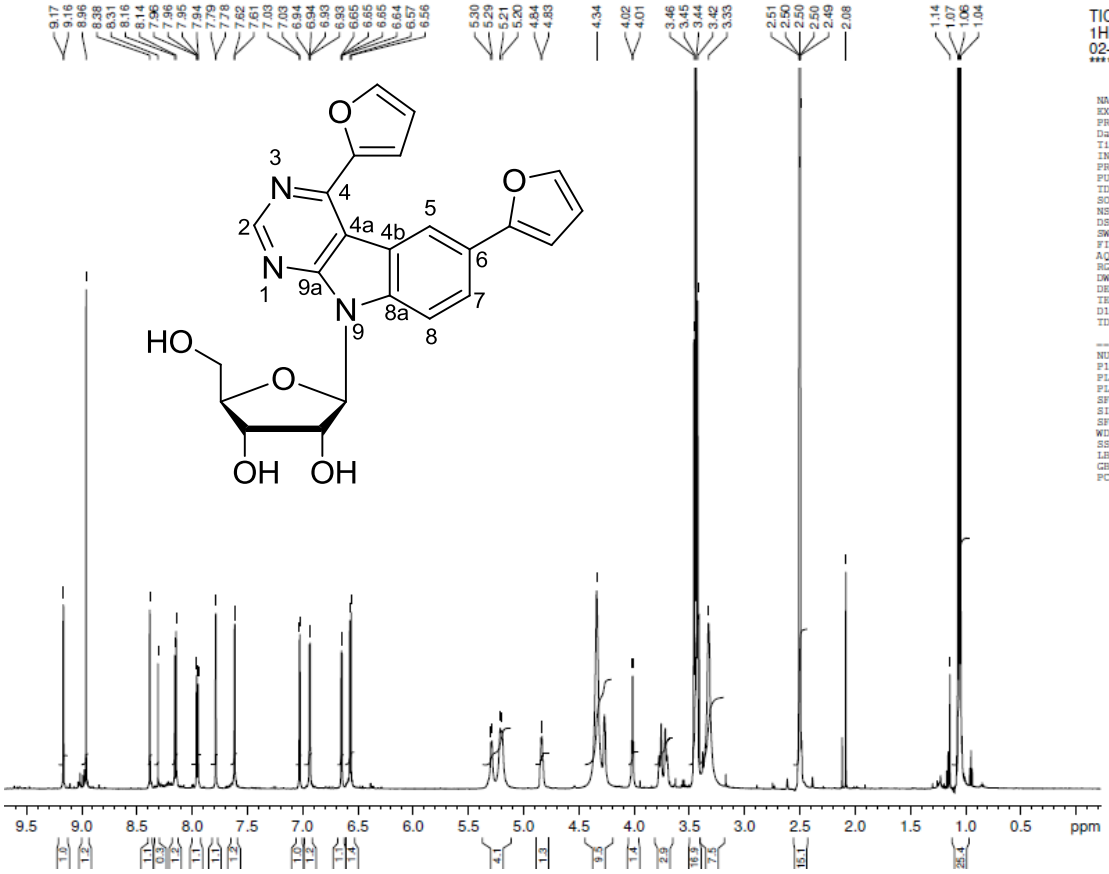

TICHY MIT-242
APT in DMSO-d6
10-08-11 LS
45032

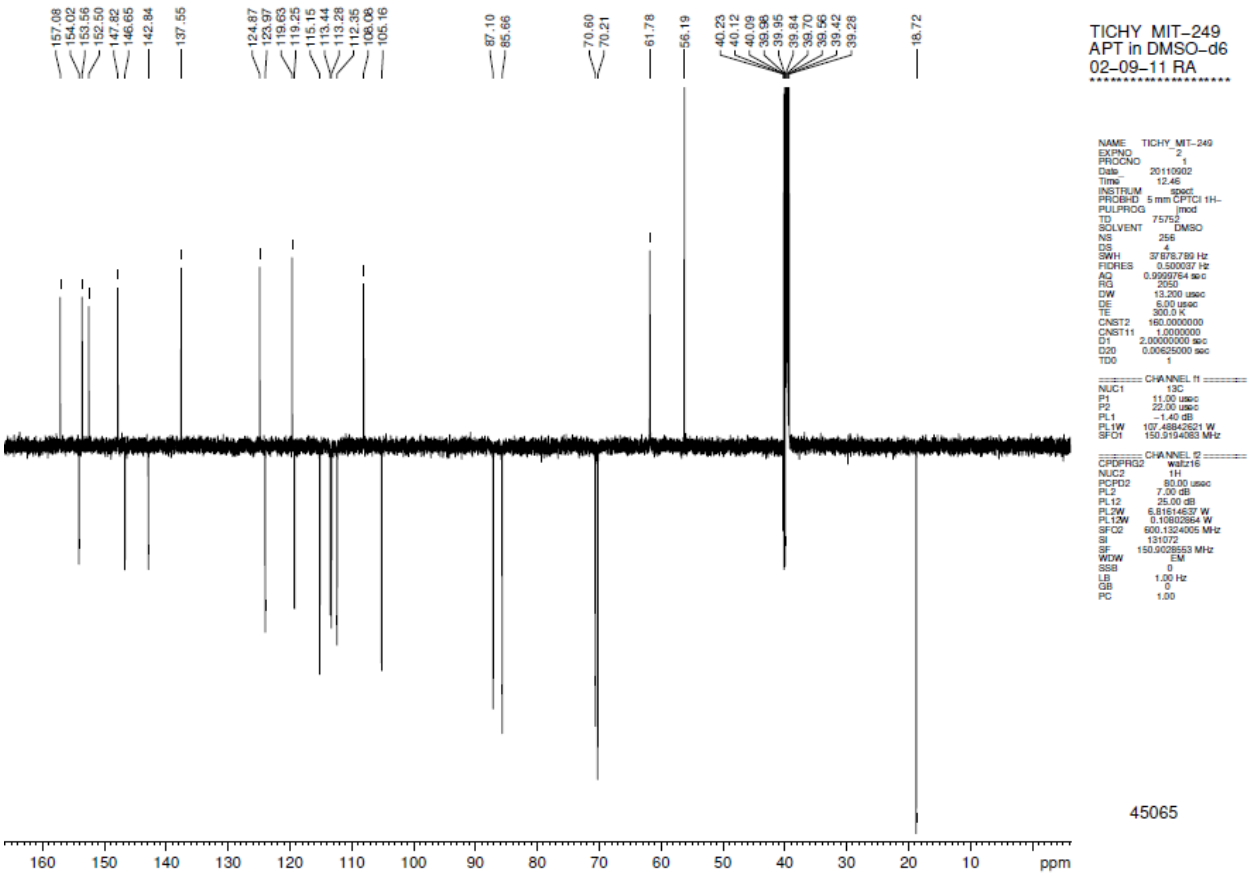
20f


TICHY_MIT-235+237
1H NMR in DMSO-d6
29-07-11 LS
45063
ppm

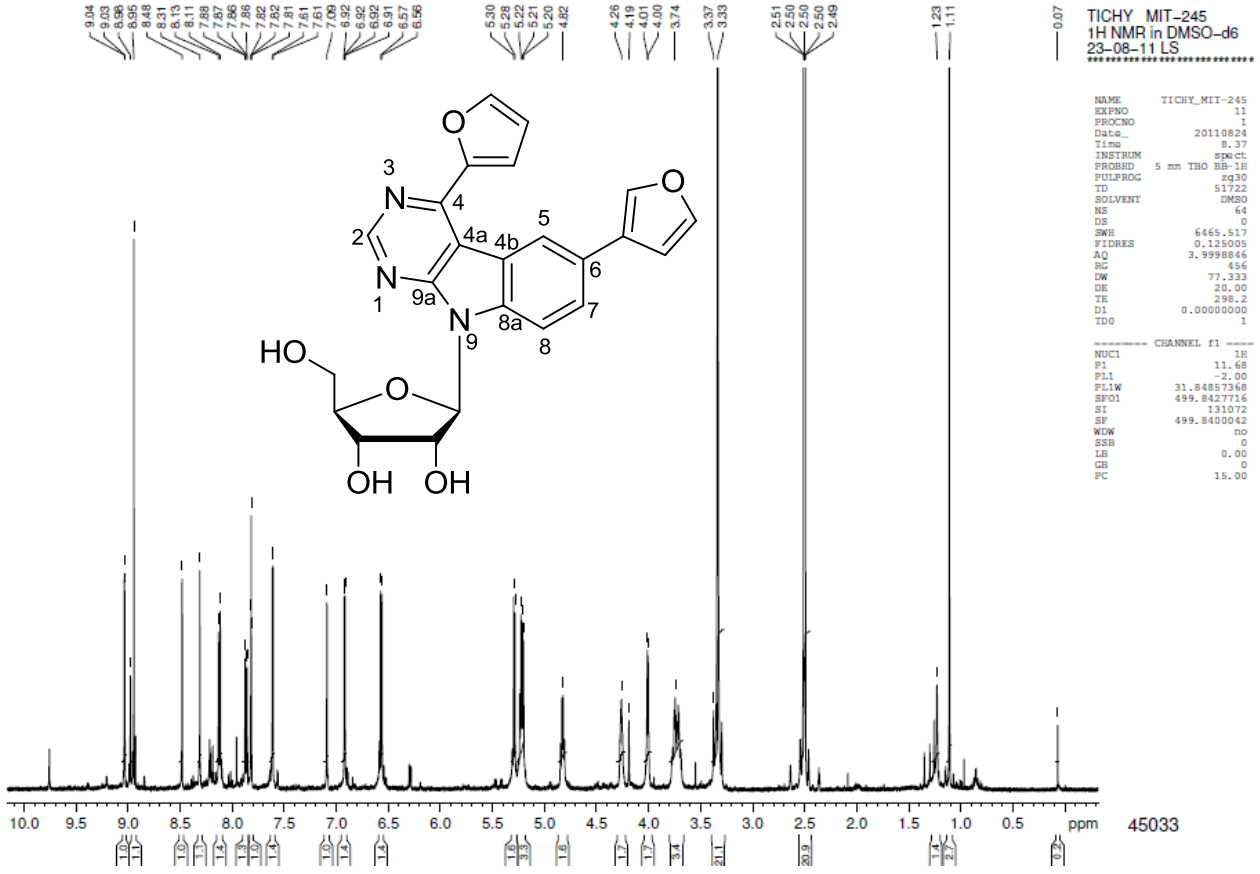

TICHY_MIT-235+237
APT in DMSO-d6
29-07-11 LS
45063
ppm

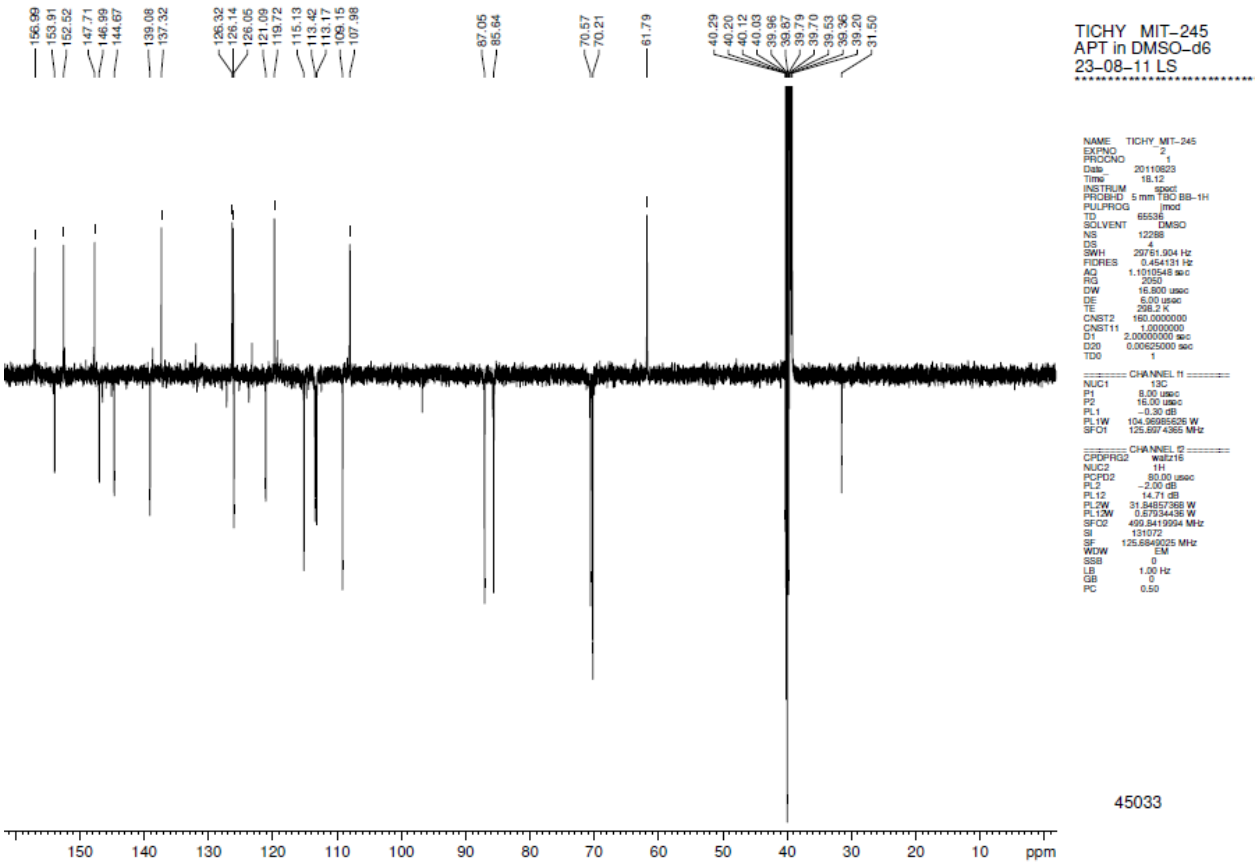
21a


TICHY_MIT-249
1H NMR in DMSO-d6
02-09-11 RA
45065
ppm

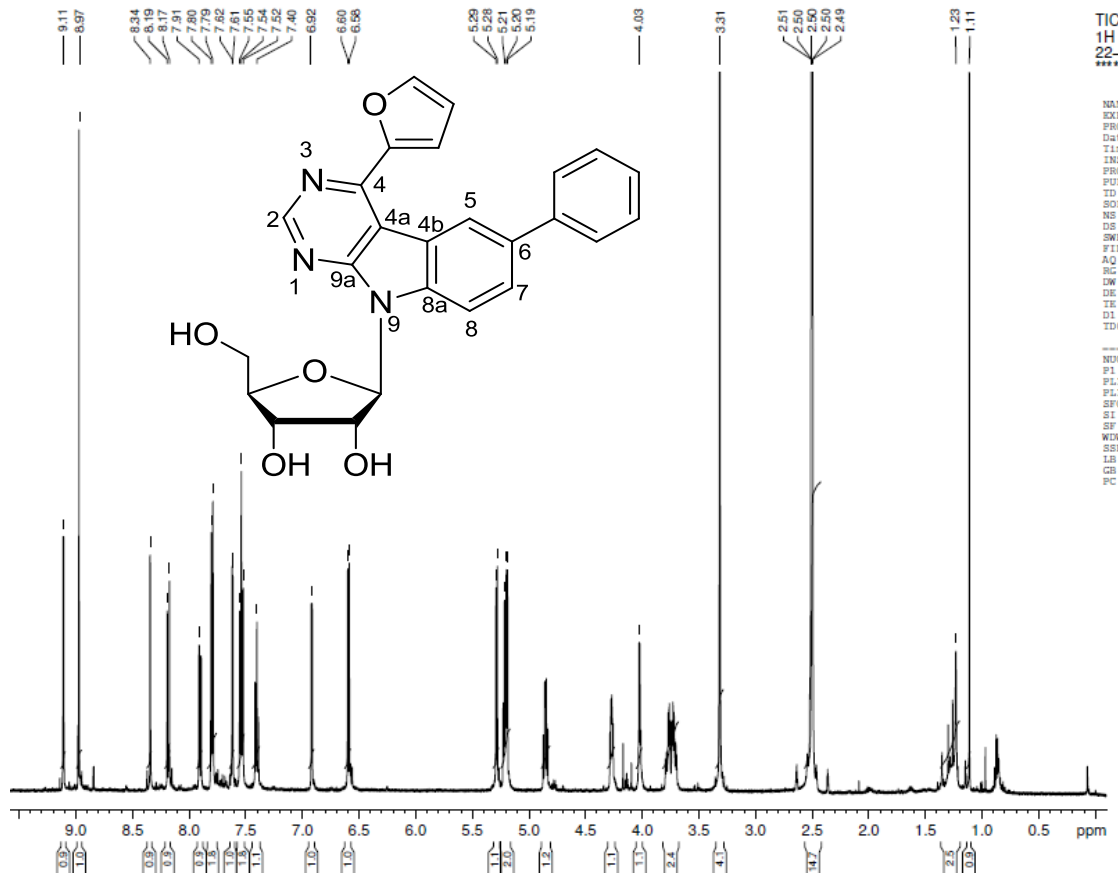

TICHY_MIT-249
APT in DMSO-d6
02-09-11 RA
45065
ppm

21b


TICHY_MIT-245
1H NMR in DMSO-d6
23-08-11 LS
45033
ppm


TICHY_MIT-245
APT in DMSO-d6
23-08-11 LS
45033
ppm

21f

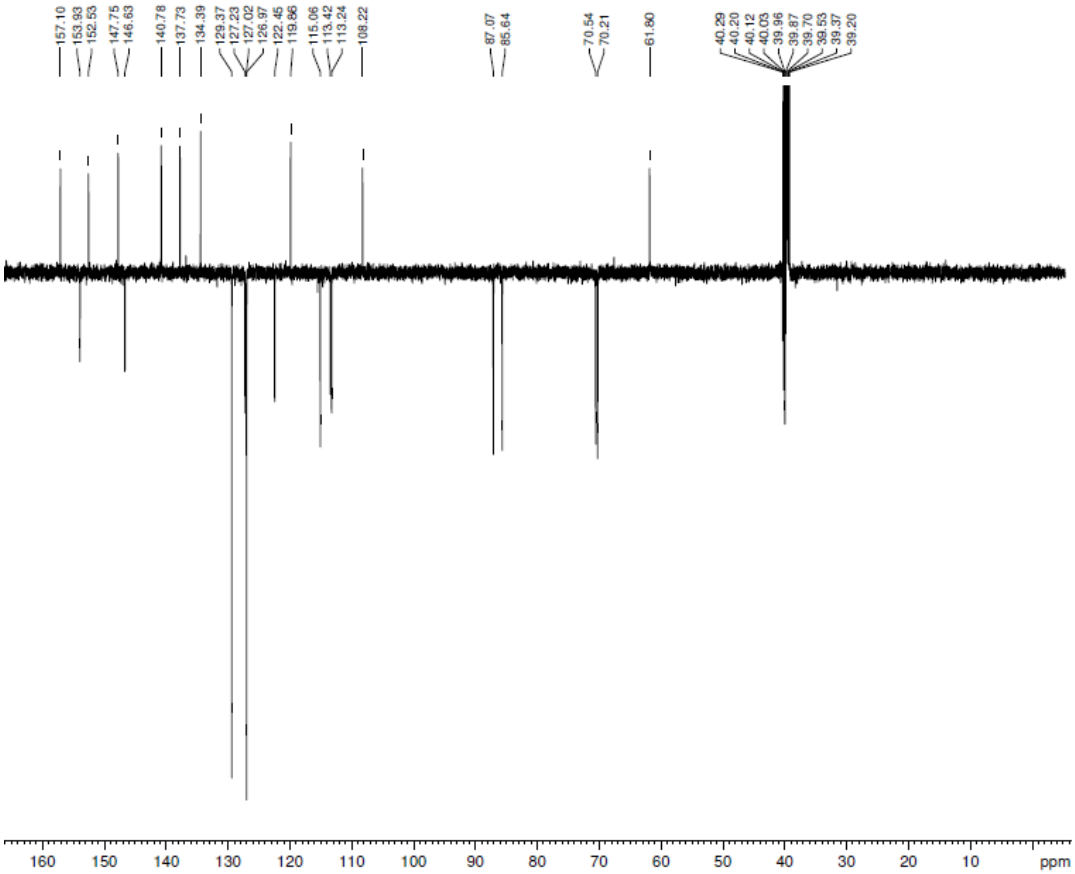


TICHY MIT-247
1H NMR in DMSO-d6
22-08-11 LS

NAME	TICHY_MIT-247
EXPNO	1
PROCNO	1
Date_	20110822
Time	17.34
INSTRUM	spect
PROBHD	5 mm TXI 1H-13
PULPROG	zg30
TD	71222
SOLVENT	DMSO
NS	32
DS	0
SWH	7122.507
FIDRES	0.100004
AQ	4.9999046
RG	12.7
DW	70.200
DE	6.00
TE	300.0
D1	1.00000000
TD0	1

CHANNEL f1

NUC1	1H
P1	9.00
PL1	3.00
PL1W	4.28034639
SFO1	499.9534565
SI	131072
SF	499.9499986
WDW	no
SSB	0
LB	0.00
GB	0
PC	10.00



TICHY MIT-247
APT in DMSO-d6
22-08-11 LS

NAME	TICHY_MIT-247
EXPNO	2
PROCNO	1
Date	20110822
Time	17.56
INSTRUM	spect
PROBHD	5 mm TXI 1H-13
PULPROG	jmod
TD	65536
SOLVENT	DMSO
NS	10240
DS	4
SWH	31446.541 Hz
FIDRES	0.479836 Hz
AQ	1.0420883 sec
RG	23170.5
DW	15.900 usec
DE	6.50 usec
TE	300.0 K
CNST2	160.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00625000 sec
TD0	1

CHANNEL f1

NUC1	13C
P1	14.50 usec
P2	29.00 usec
PL1	0.00 dB
PL1W	67.92093048 W
SFO1	125.7276125 MHz

CHANNEL f2

CPDPRG2	waltz16
NUC2	1H
PCPD2	60.00 usec
PL2	3.00 dB
PL12	19.48 dB
PL2W	4.28034639 W
PL12W	0.09526734 W
SFO2	499.9519998 MHz
SI	131072
SF	125.7125655 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00