

Supporting Information II

Synthesis and Cytotoxic and Antiviral Profiling of Pyrrolo- and Furo-fused 7-Deazapurine Ribonucleosides

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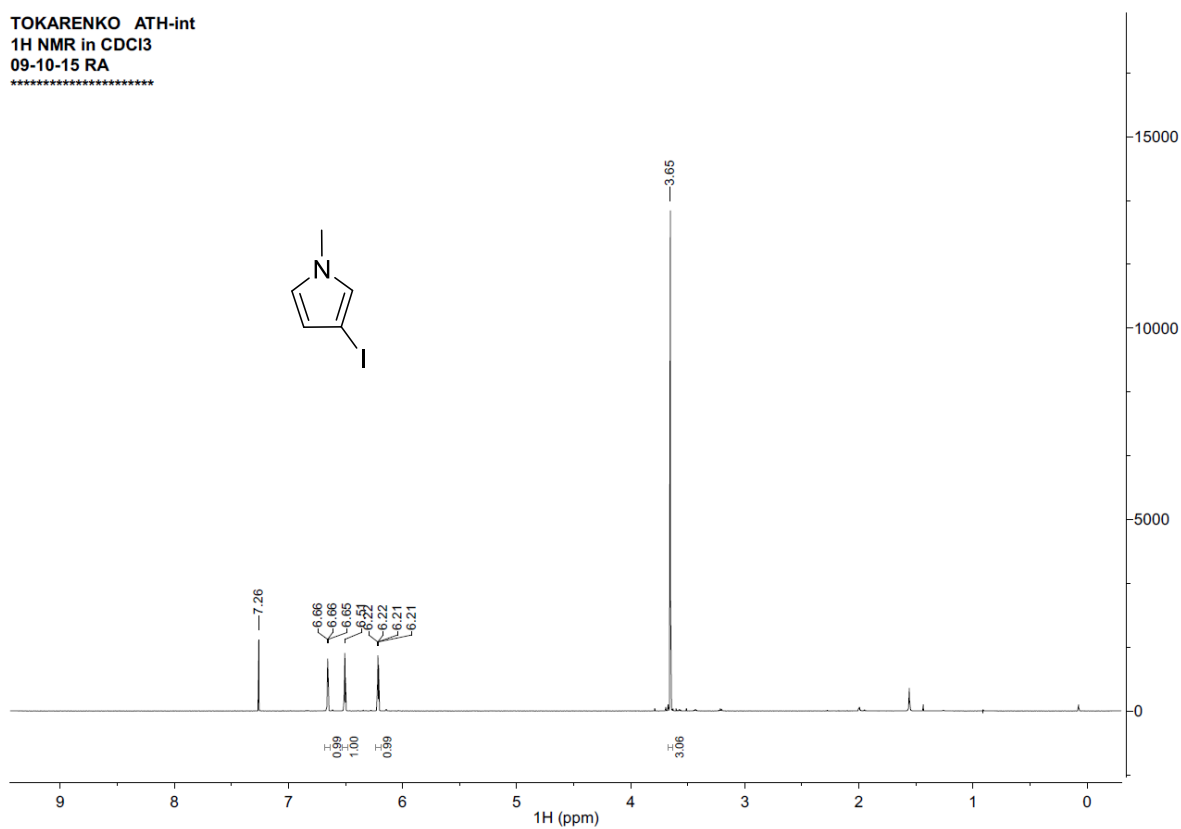
Contents:

Copies of NMR spectra

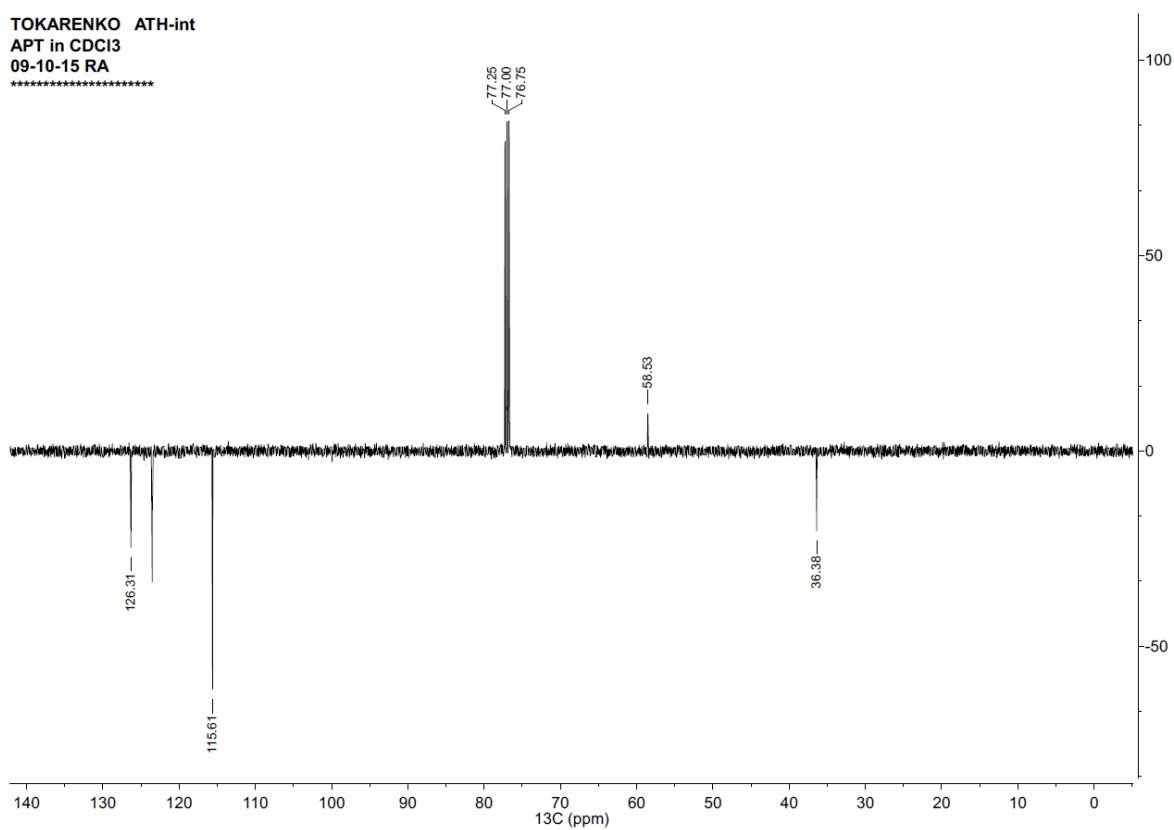
Copies of NMR spectra

NMR spectra of 3-iodo-1-methyl-1*H*-pyrrole

TOKARENKO ATH-int
1H NMR in CDCl₃
09-10-15 RA



TOKARENKO ATH-int
APT in CDCl₃
09-10-15 RA

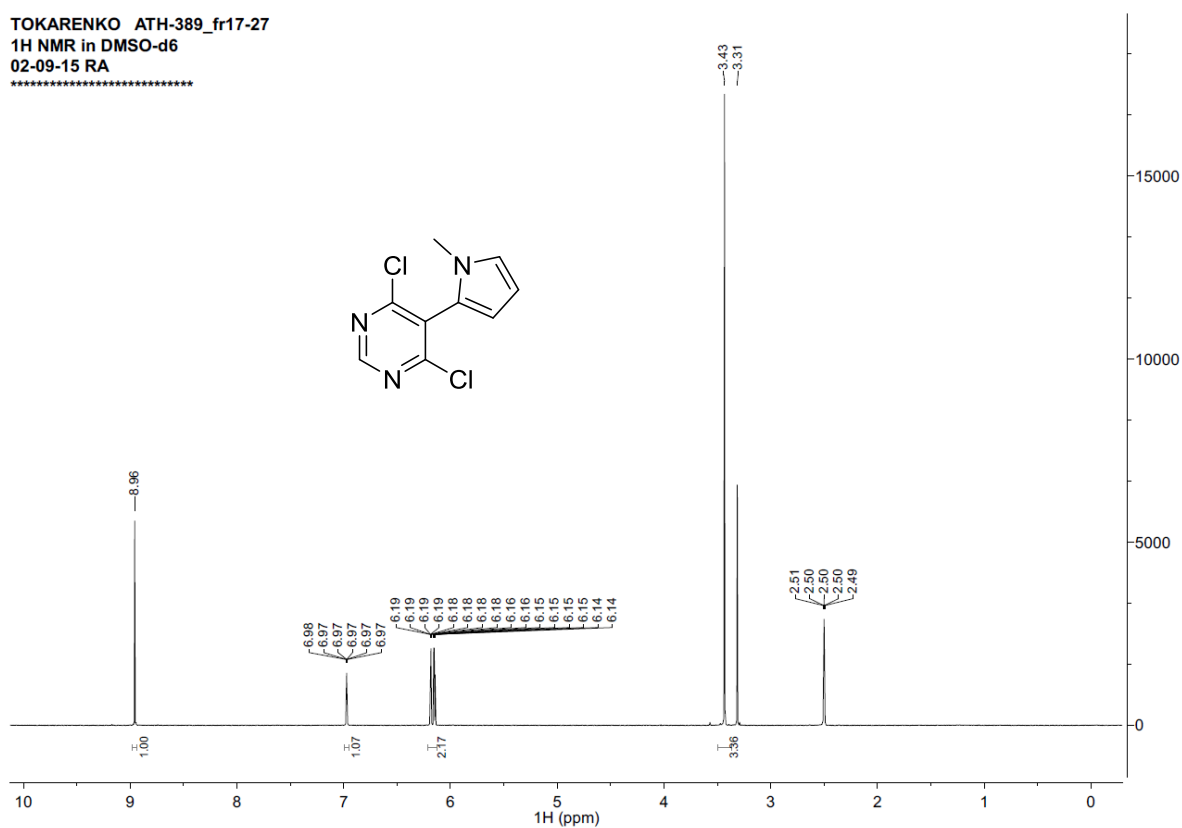


NMR spectra of compound 7

TOKARENKO ATH-389_fr17-27

¹H NMR in DMSO-d₆

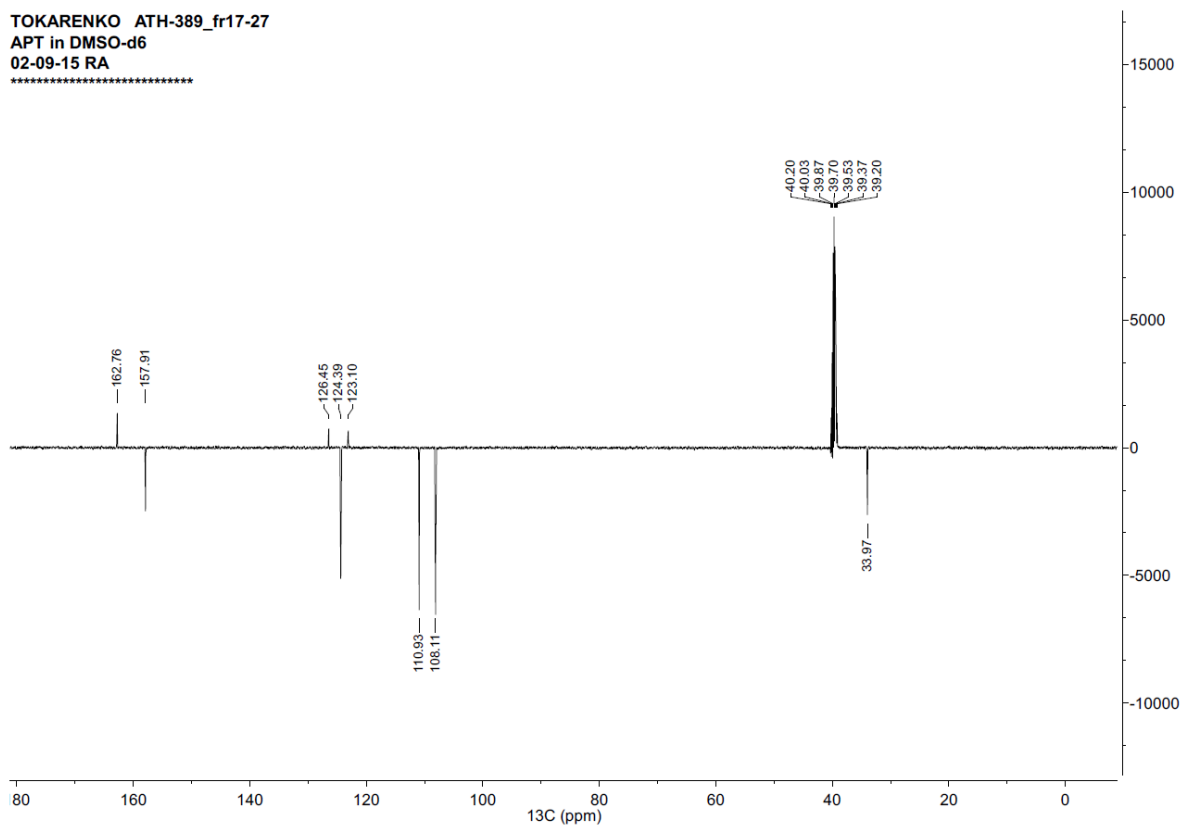
02-09-15 RA



TOKARENKO ATH-389_fr17-27

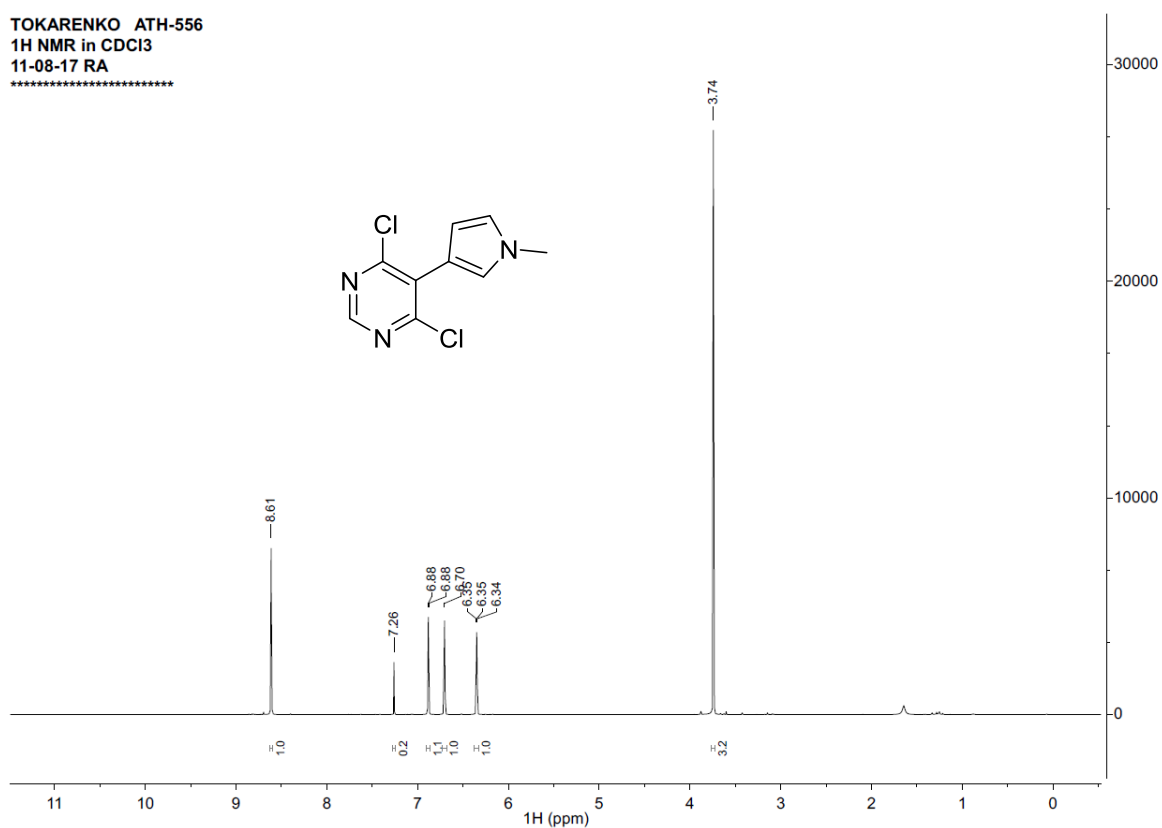
APT in DMSO-d₆

02-09-15 RA

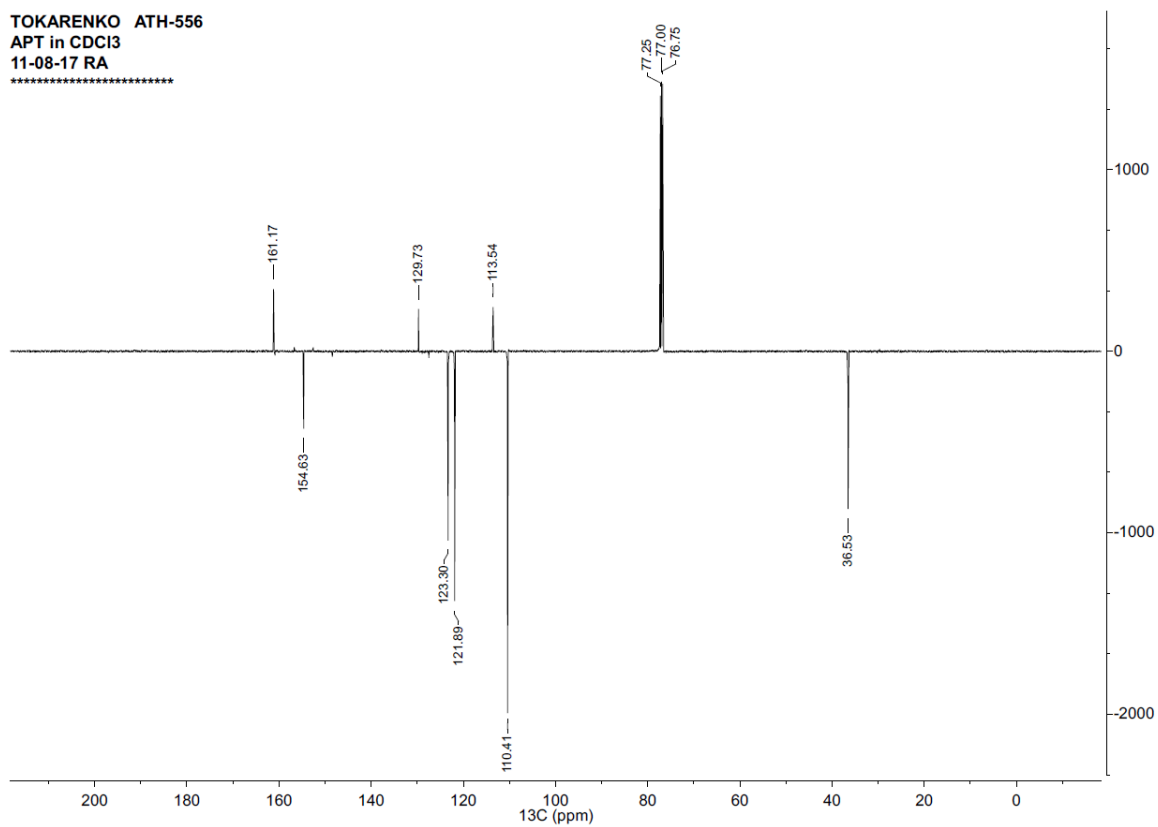


NMR spectra of compound **8**

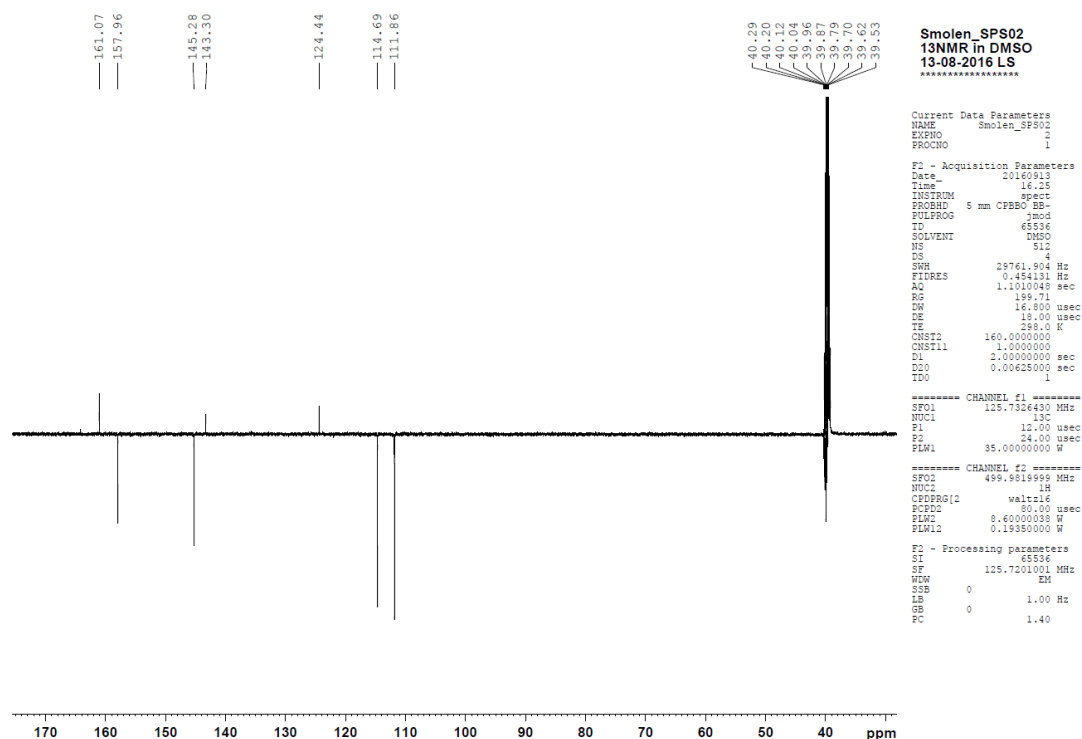
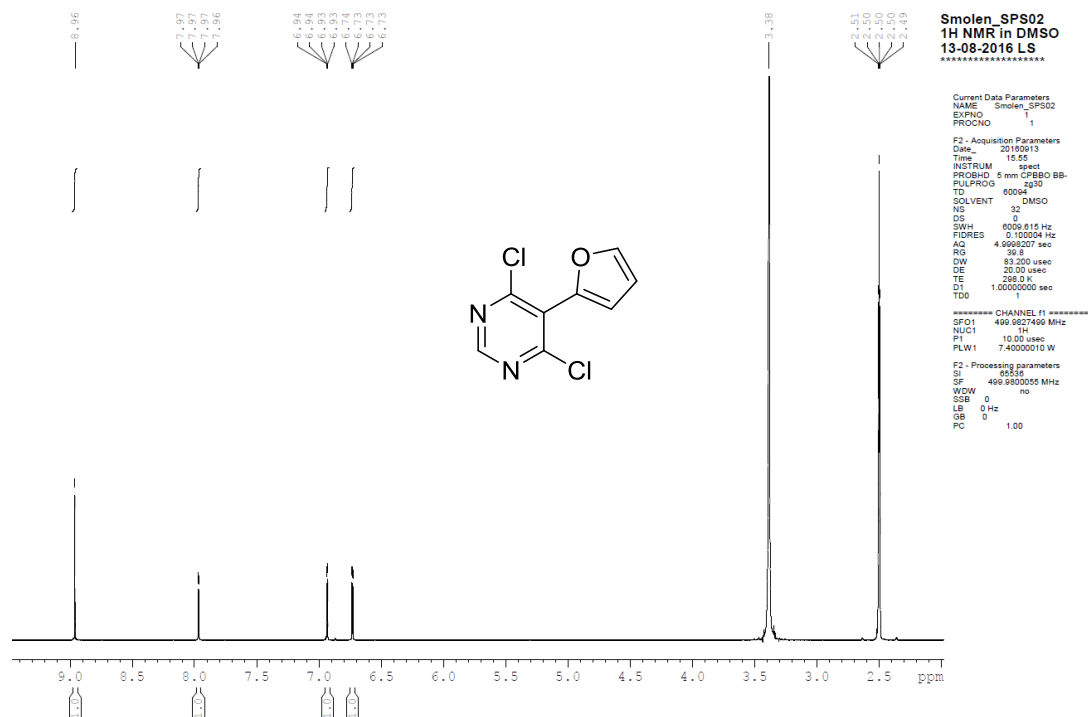
TOKARENKO ATH-556
 1H NMR in CDCl₃
 11-08-17 RA



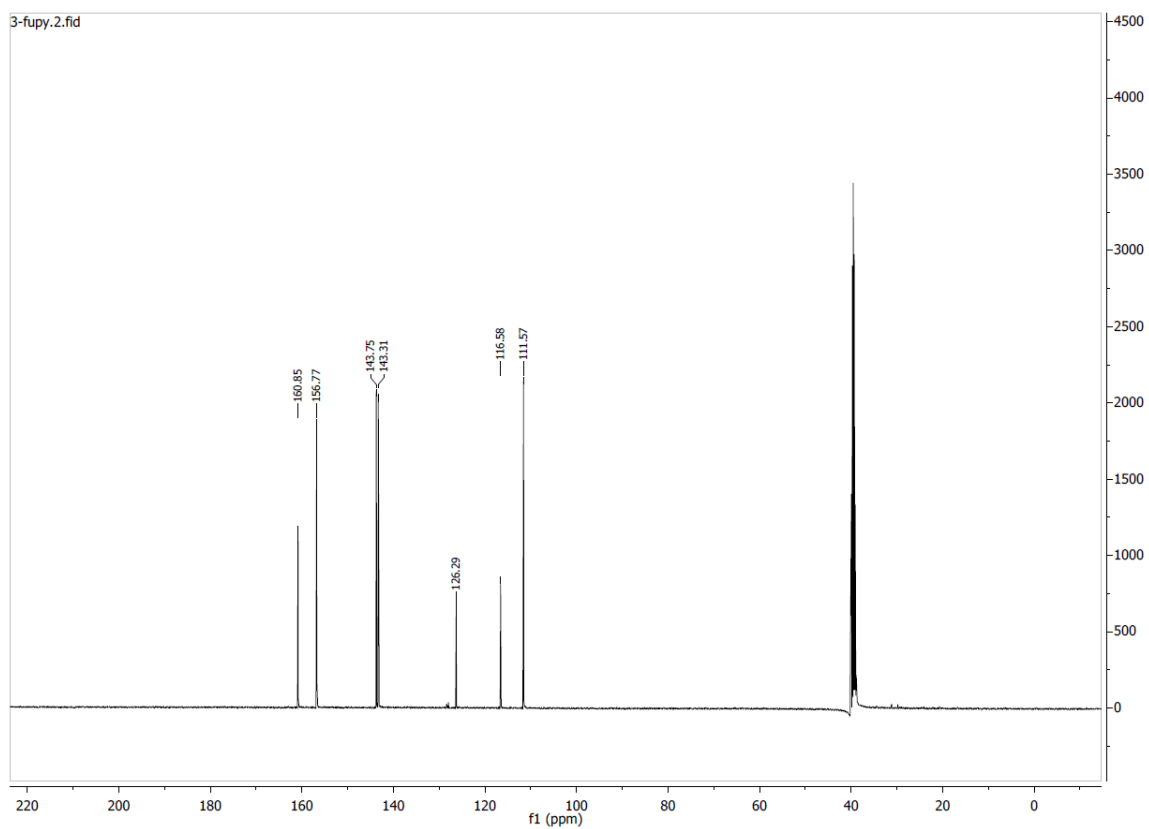
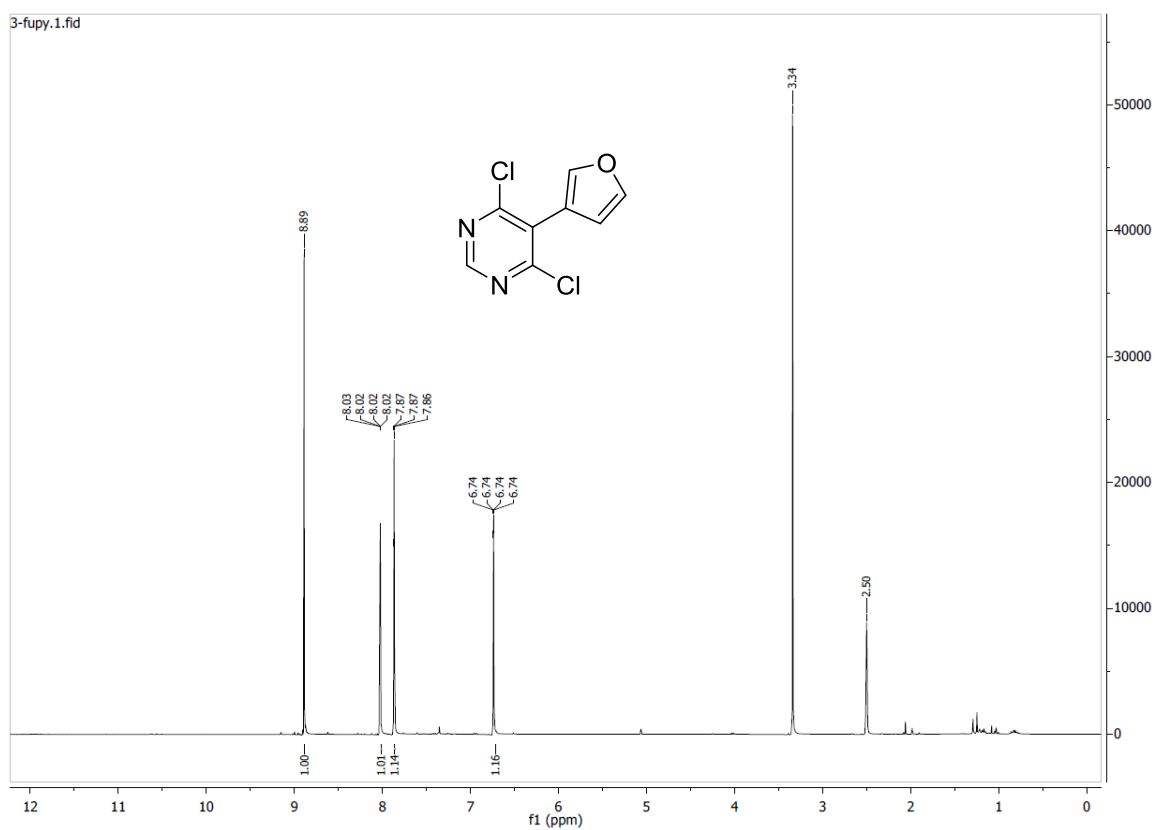
TOKARENKO ATH-556
 APT in CDCl₃
 11-08-17 RA



NMR spectra of compound **9**

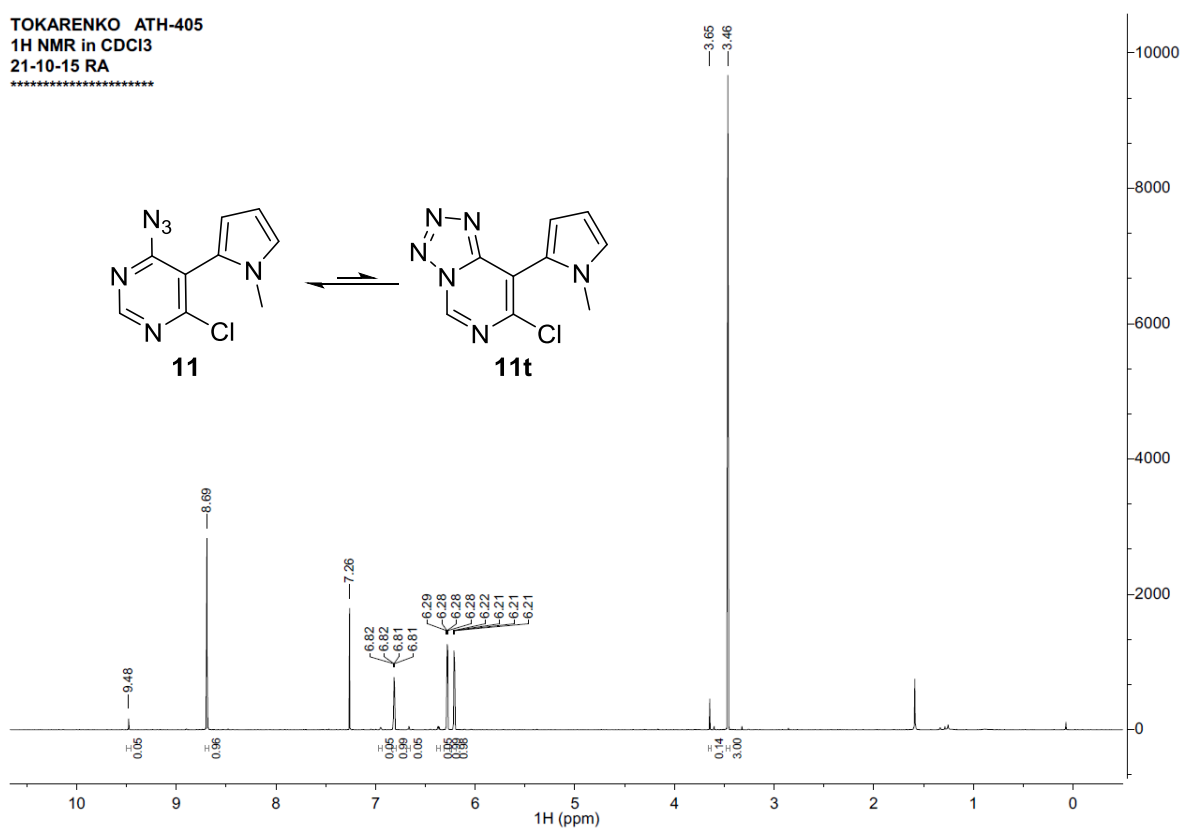


NMR spectra of compound **10**

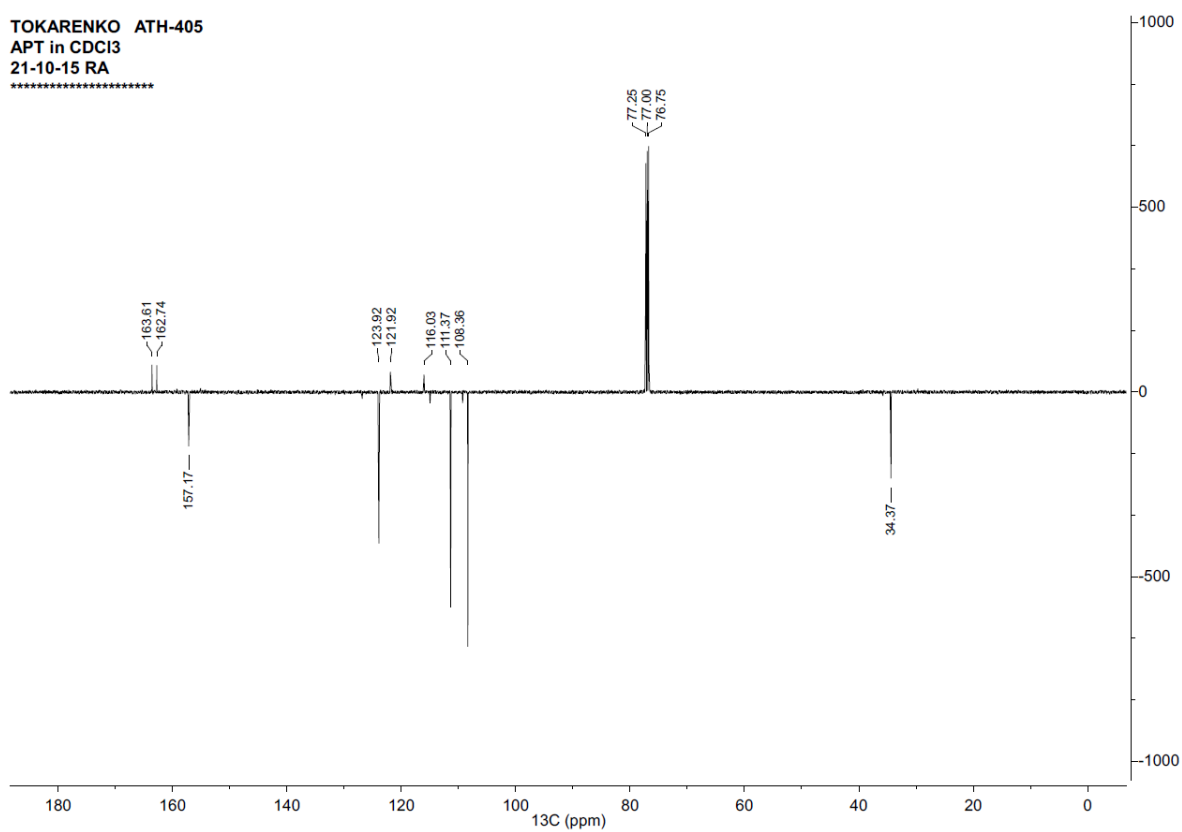


NMR spectra of compound **11** (**11t**)

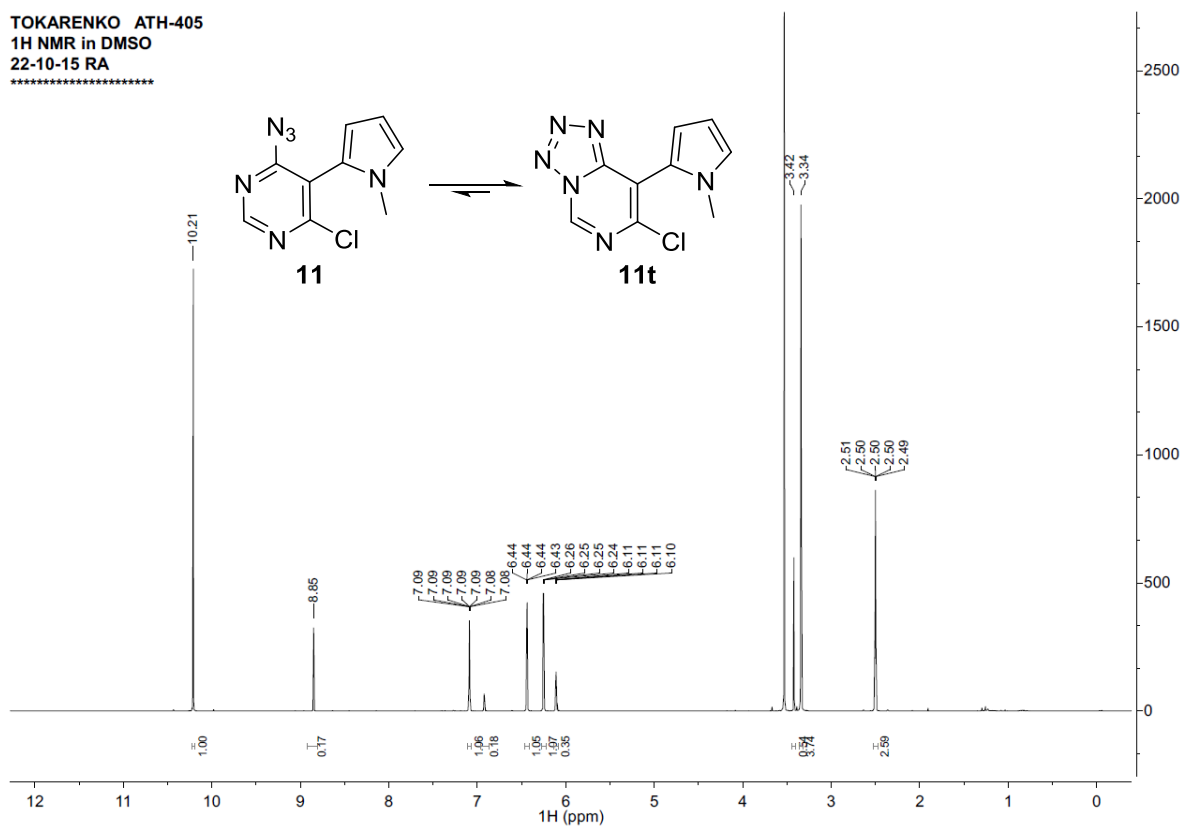
TOKARENKO ATH-405
 1H NMR in CDCl₃
 21-10-15 RA



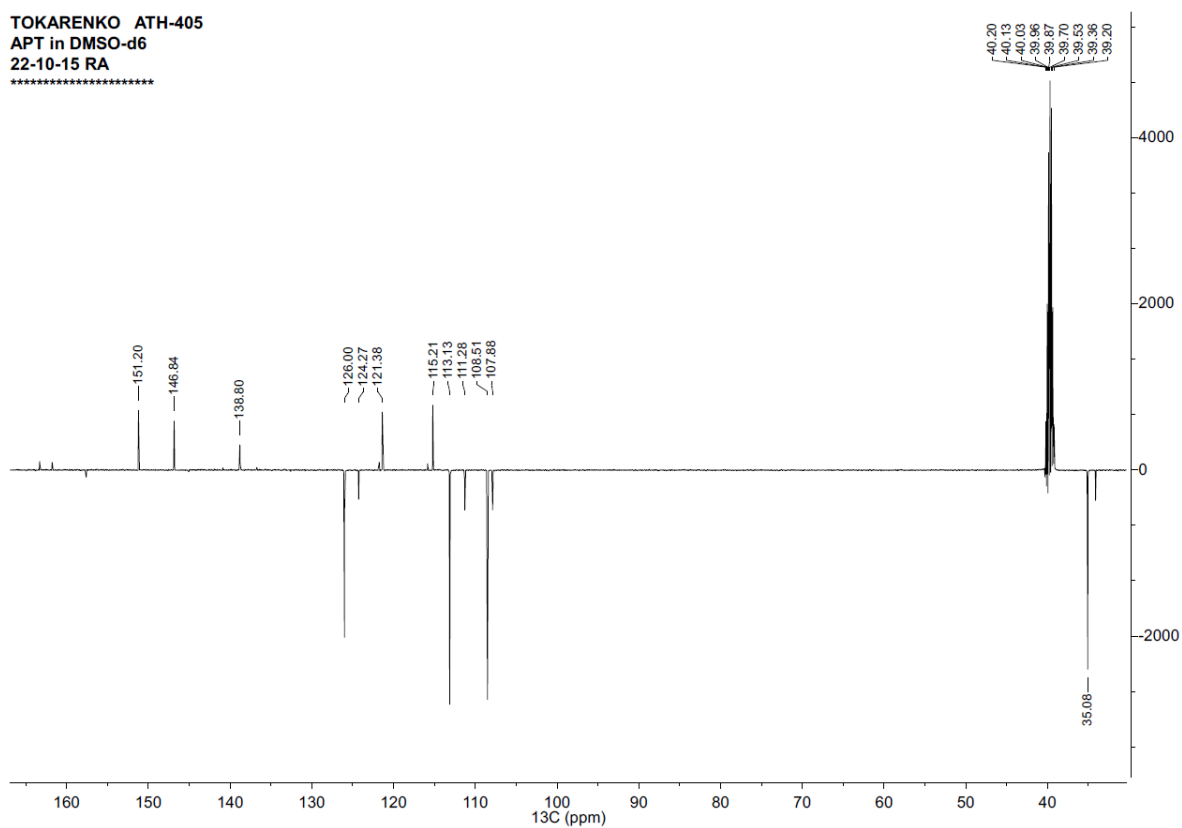
TOKARENKO ATH-405
 APT in CDCl₃
 21-10-15 RA



TOKARENKO ATH-405
 1H NMR in DMSO
 22-10-15 RA

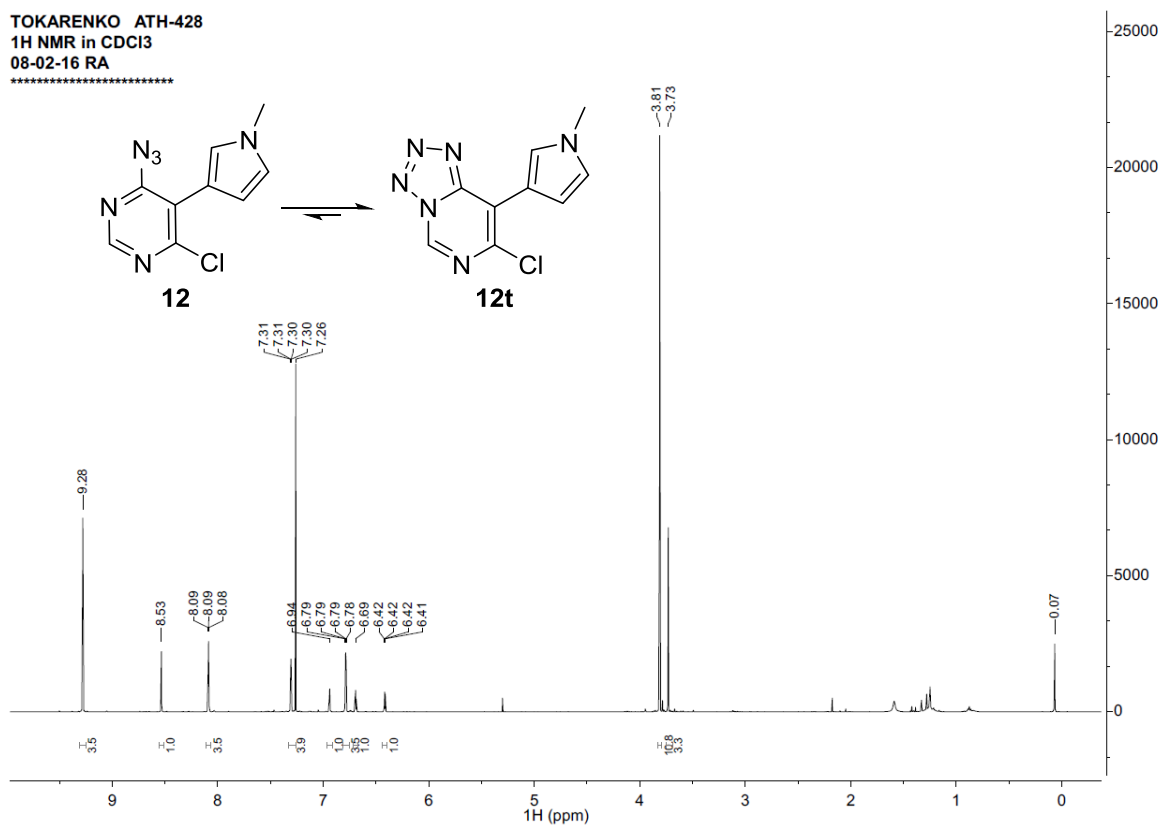


TOKARENKO ATH-405
 APT in DMSO-d6
 22-10-15 RA

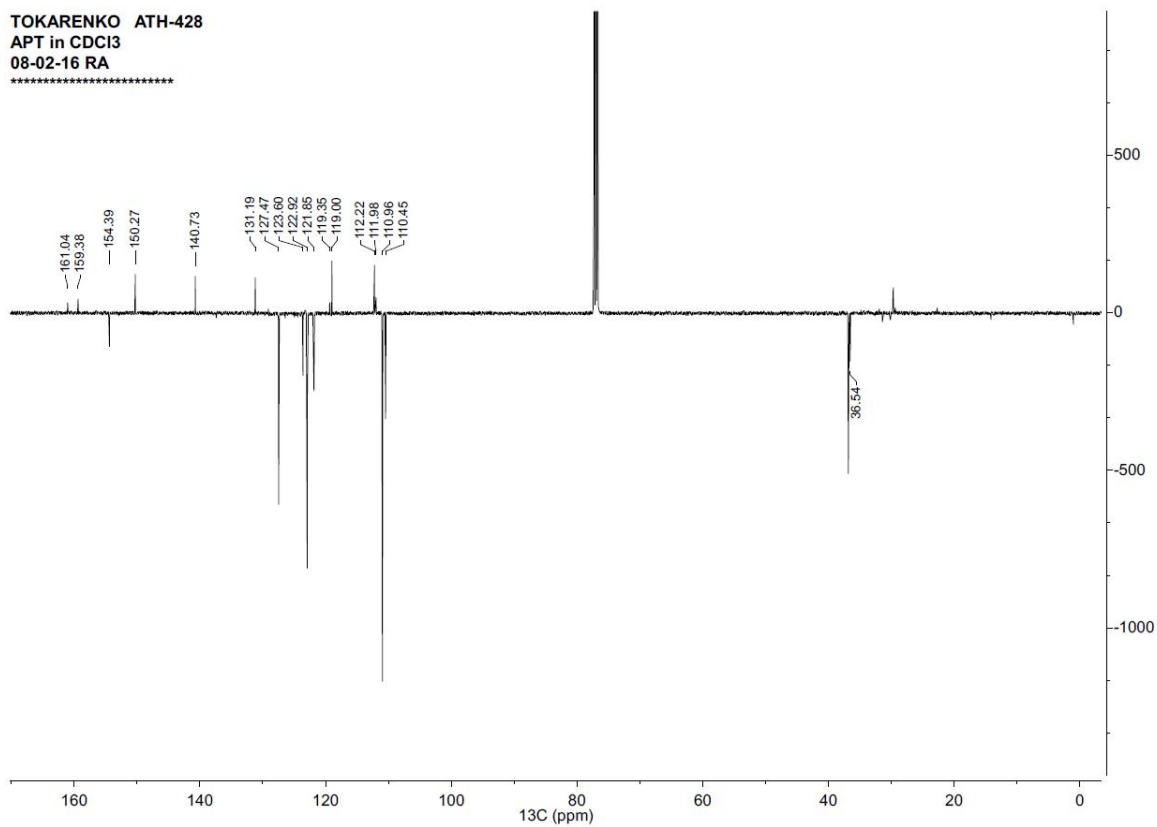


NMR spectra of compound **12** (**12t**)

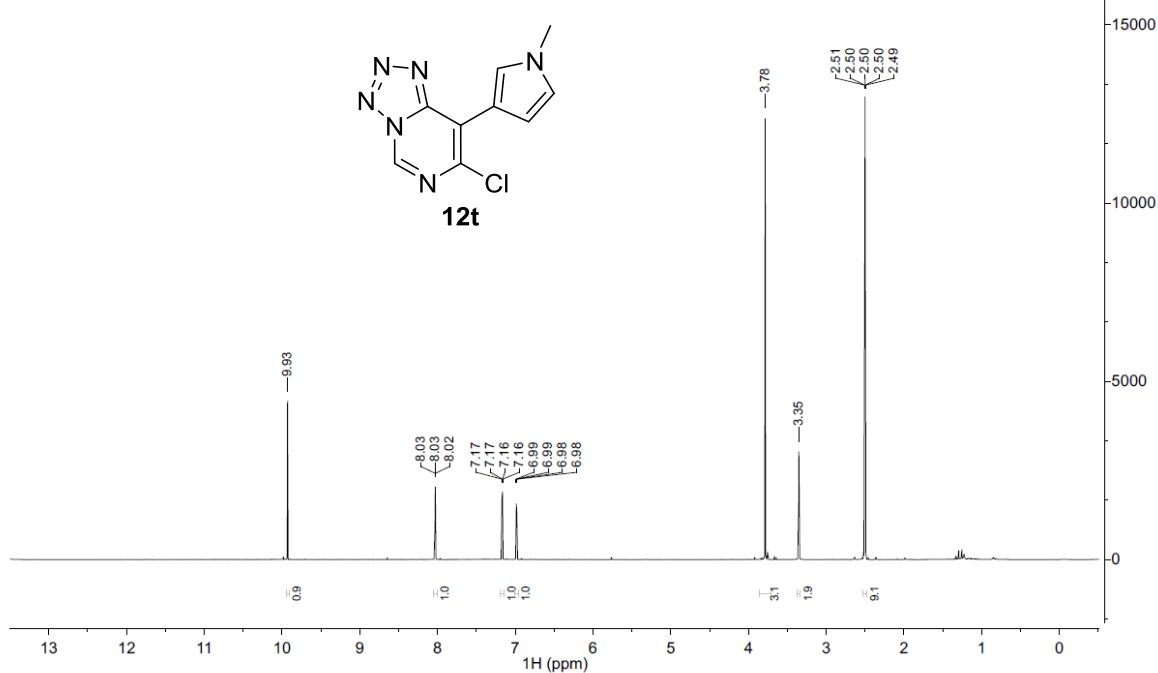
TOKARENKO ATH-428
1H NMR in CDCl₃
08-02-16 RA



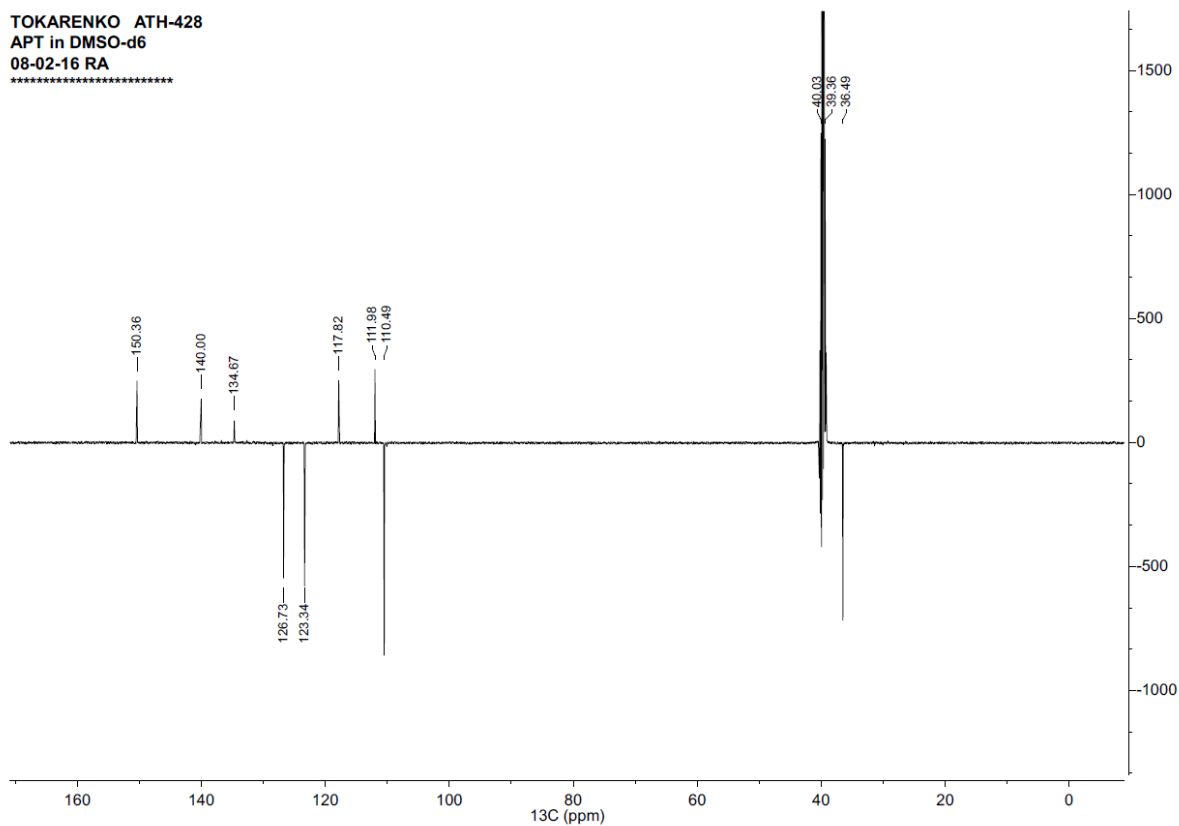
TOKARENKO ATH-428
APT in CDCl₃
08-02-16 RA



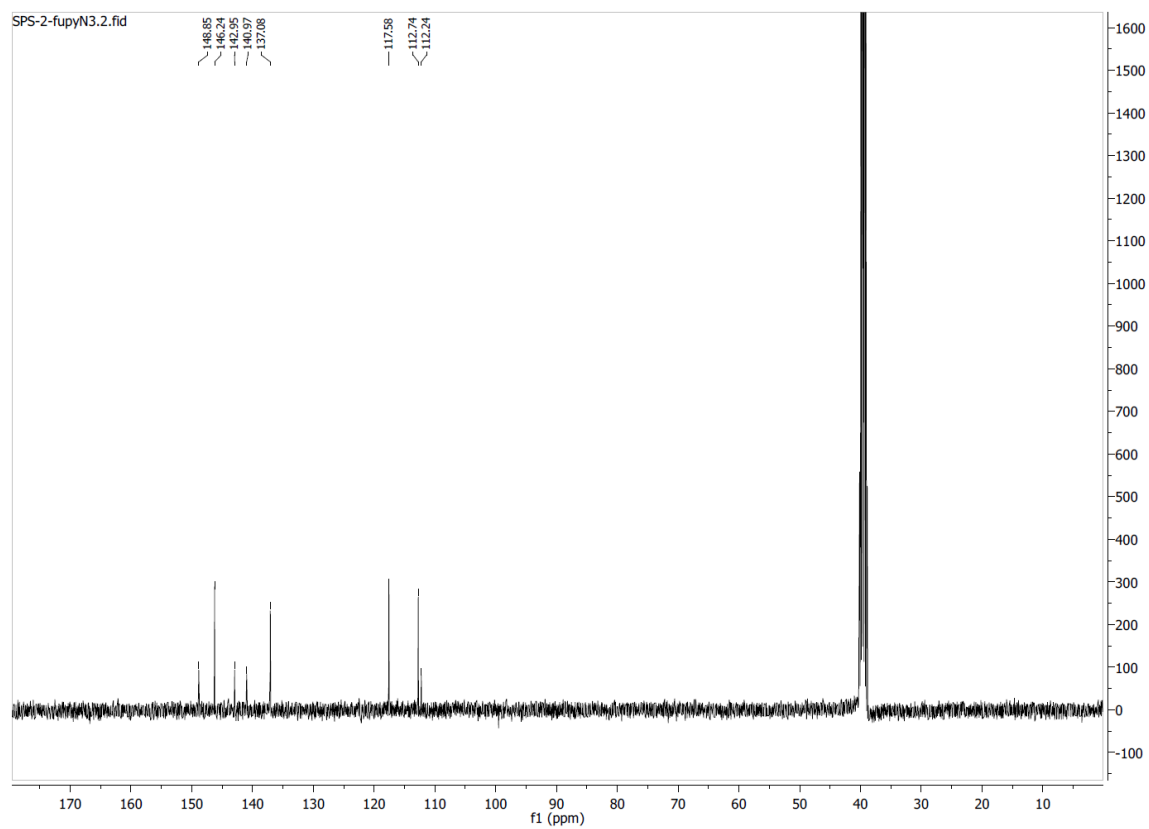
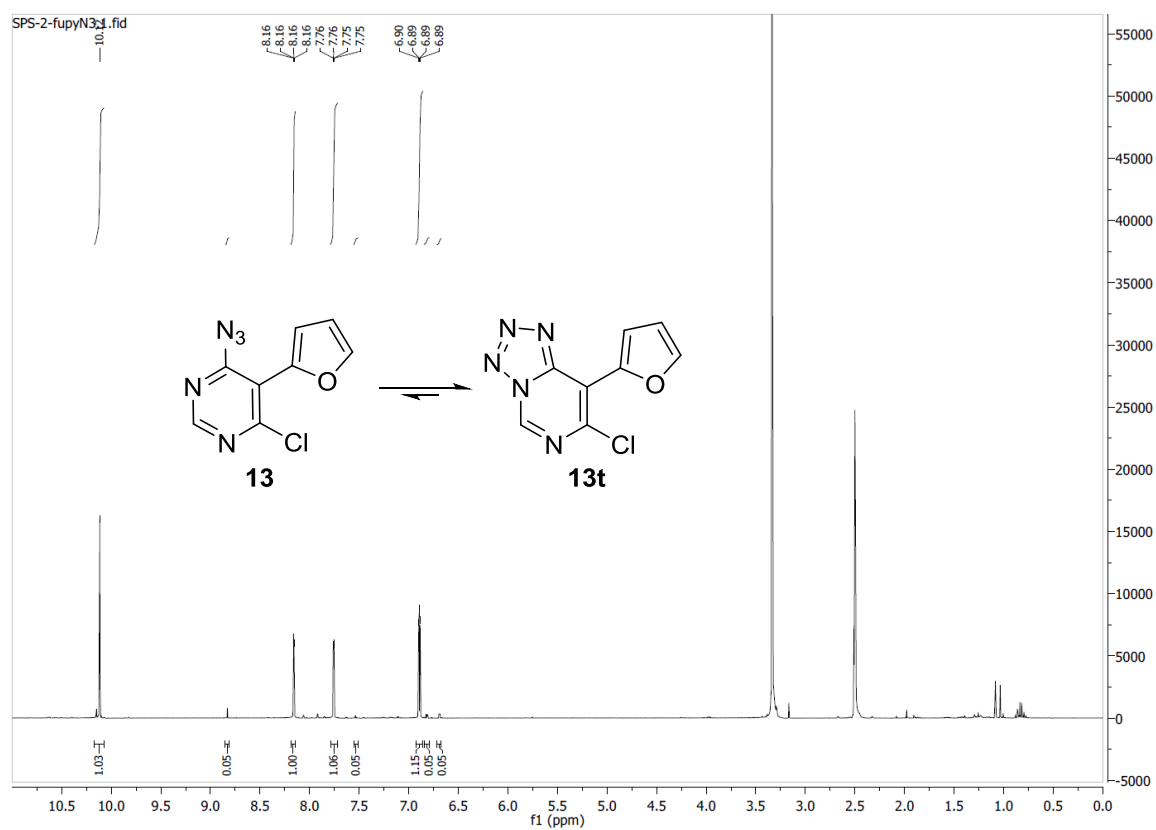
TOKARENKO ATH-428
 1H NMR in DMSO-d6
 08-02-16 RA



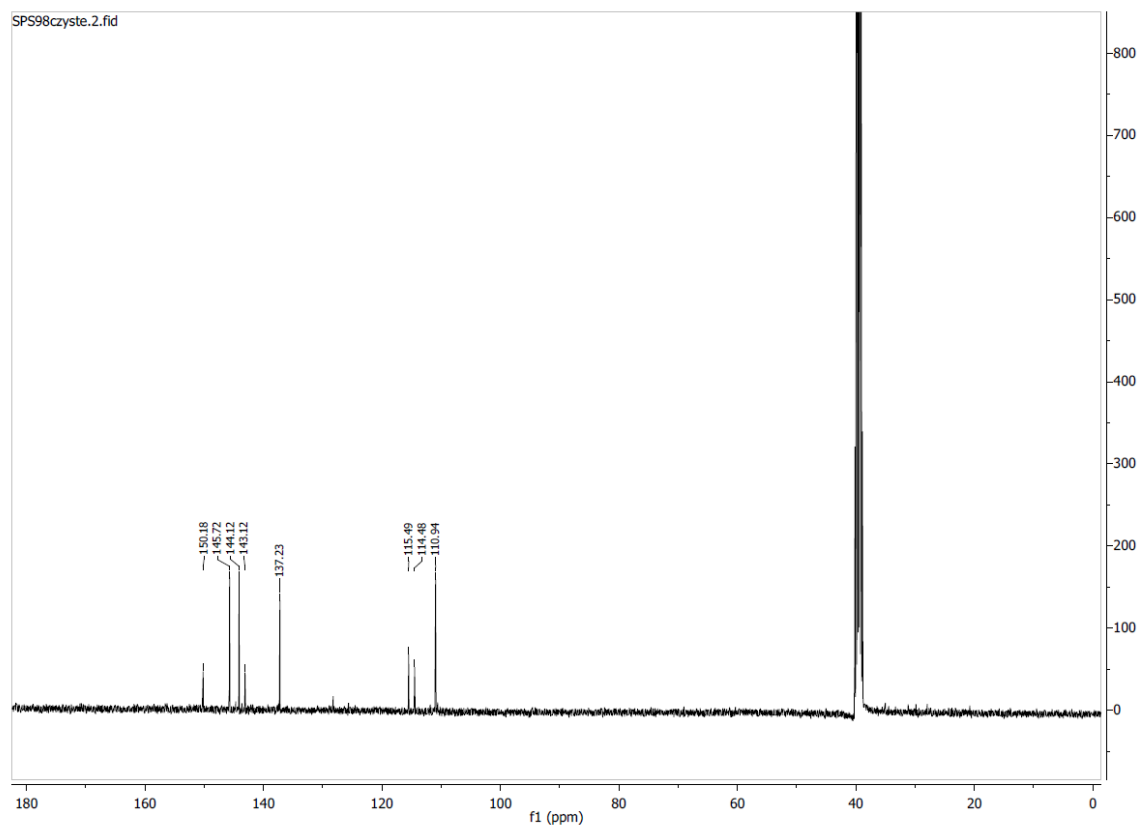
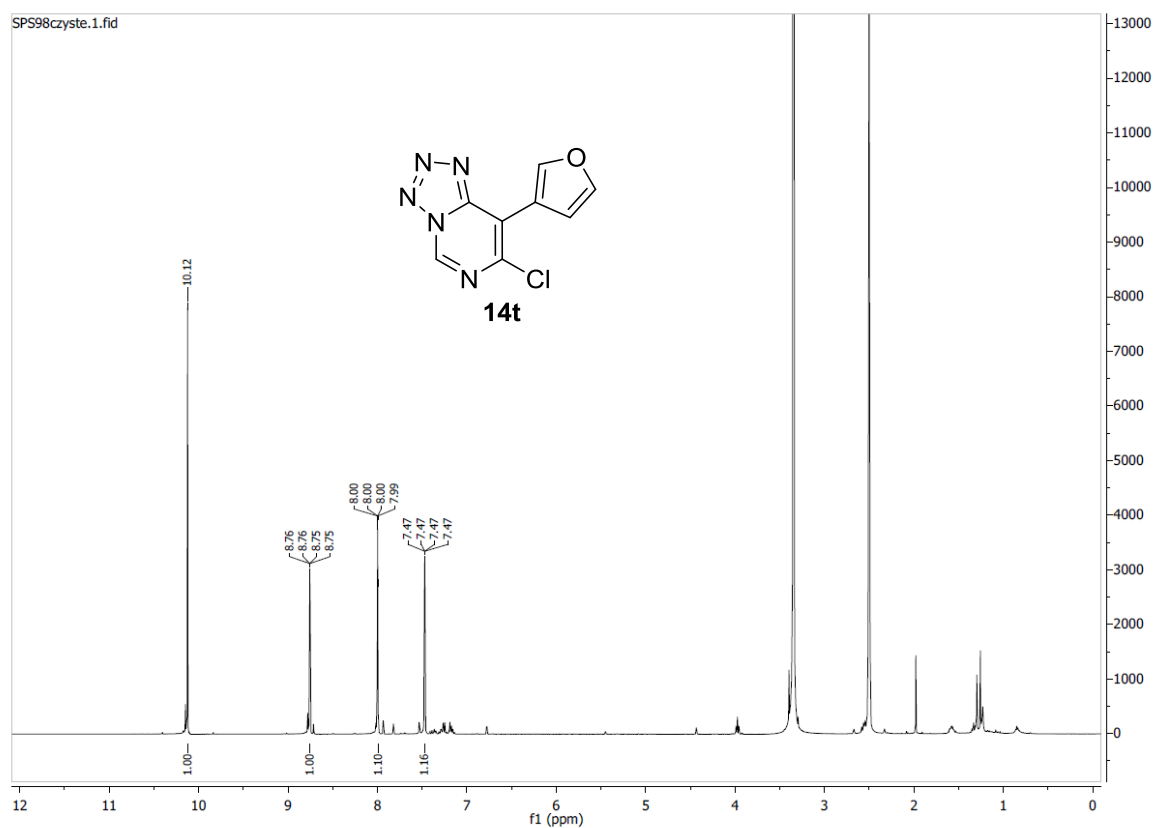
TOKARENKO ATH-428
 APT in DMSO-d6
 08-02-16 RA



NMR spectra of compound **13** (**13t**)

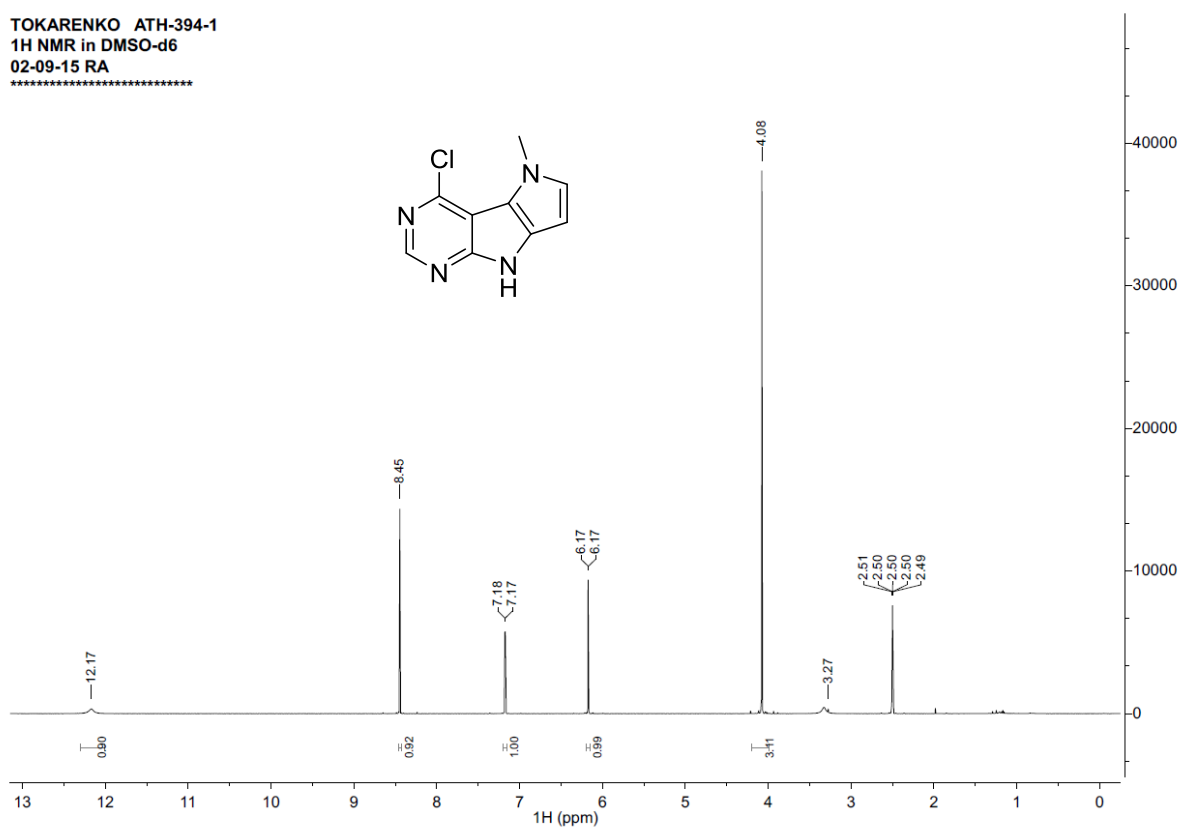


NMR spectra of compound **14** (**14t**)

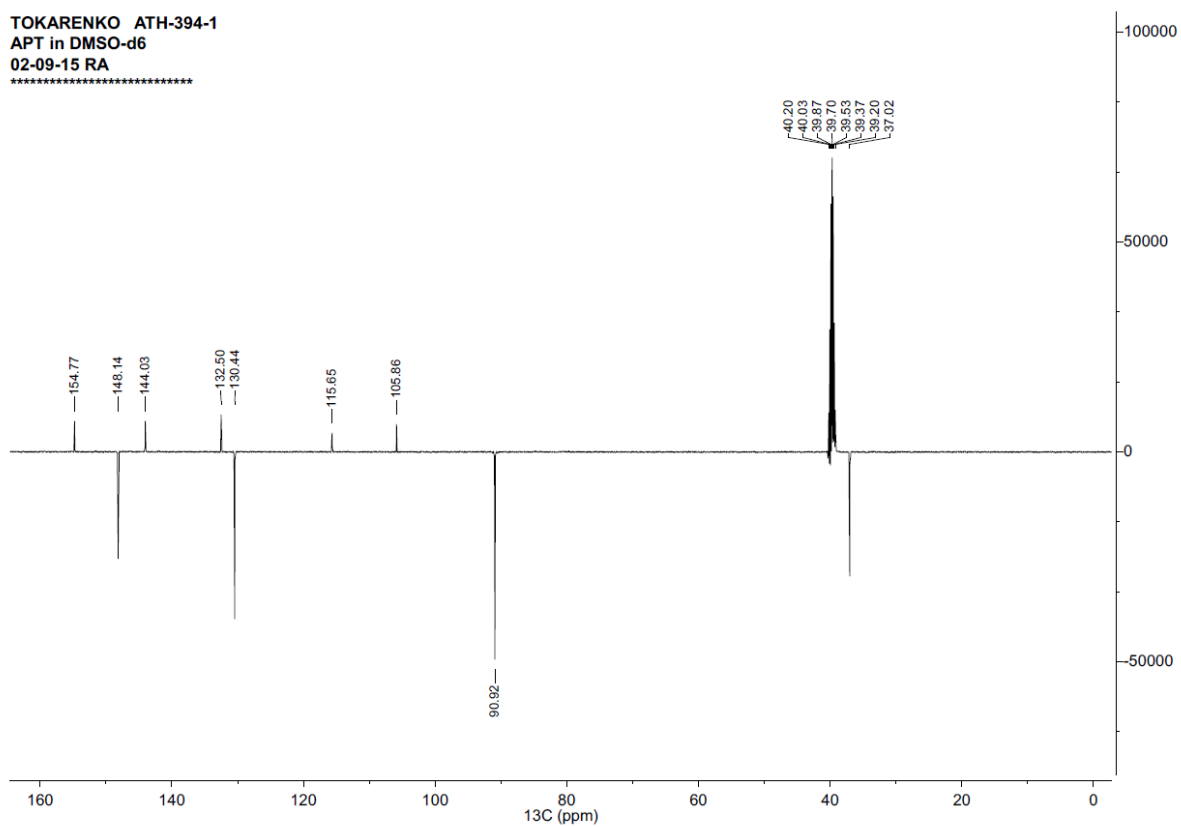


NMR spectra of compound **15**

TOKARENKO ATH-394-1
 1H NMR in DMSO-d6
 02-09-15 RA

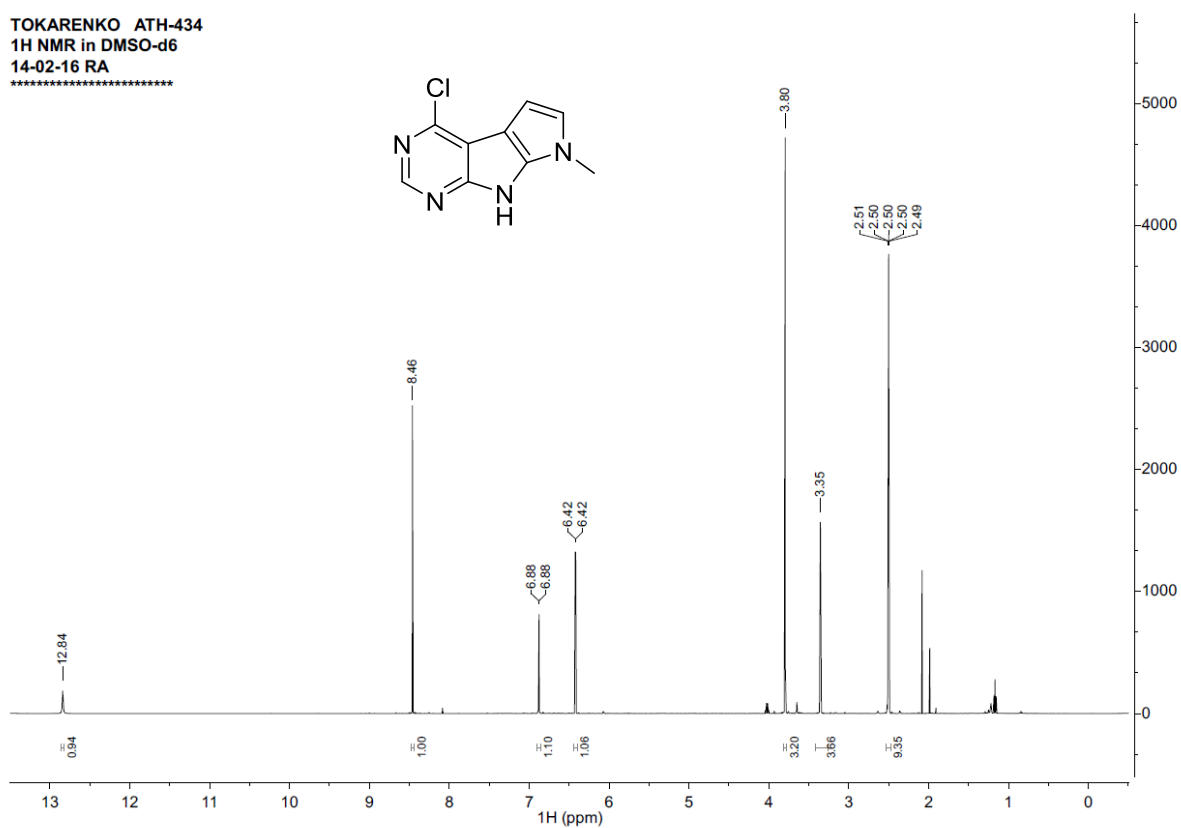


TOKARENKO ATH-394-1
 APT in DMSO-d6
 02-09-15 RA

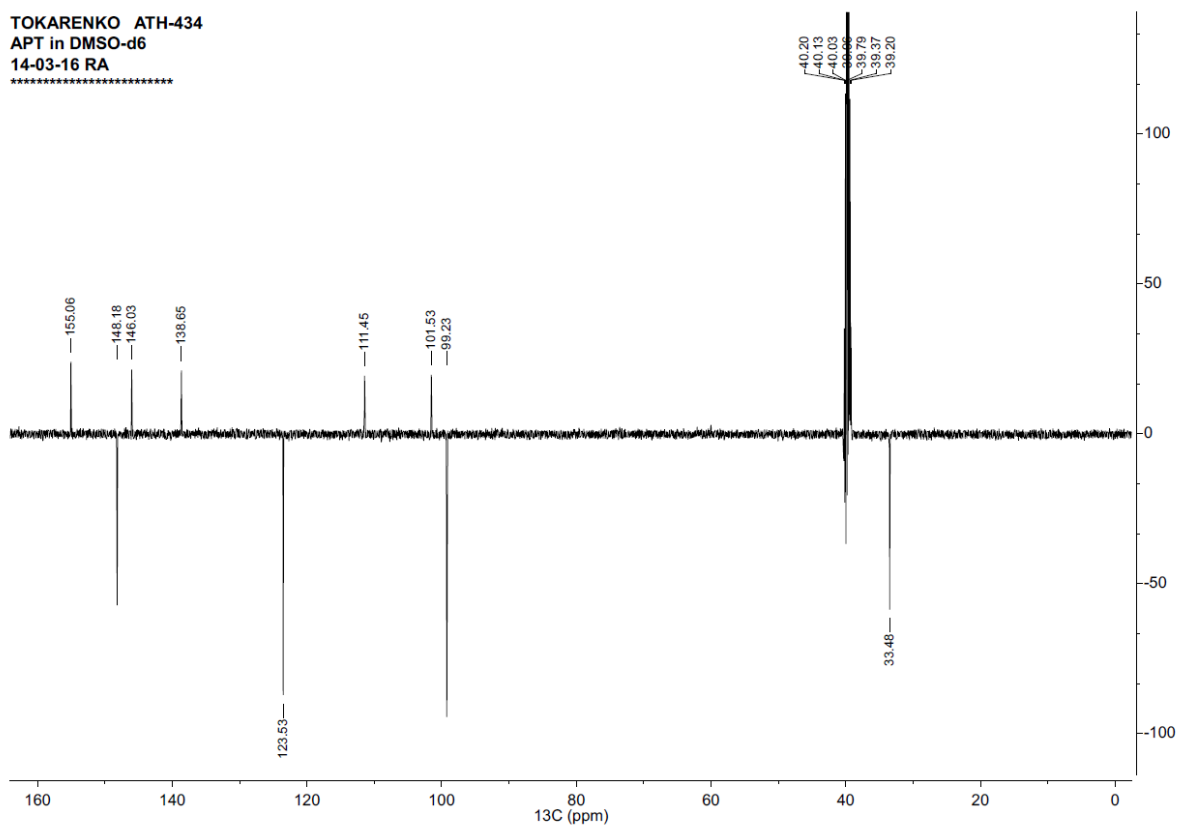


NMR spectra of compound **16**

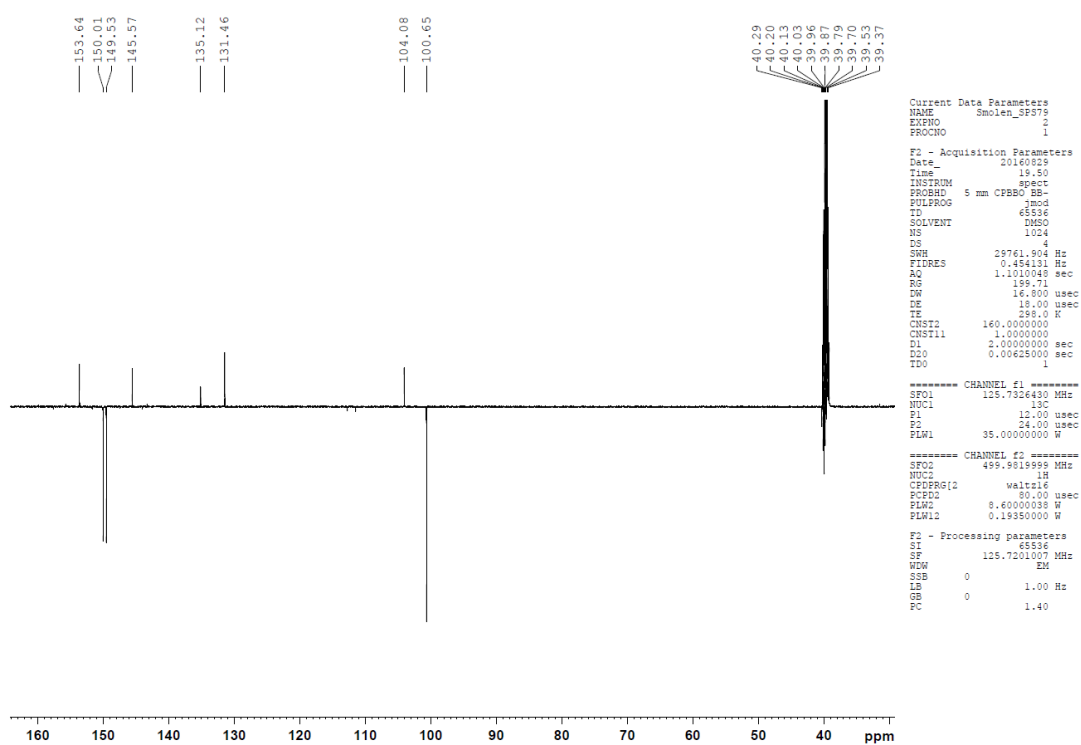
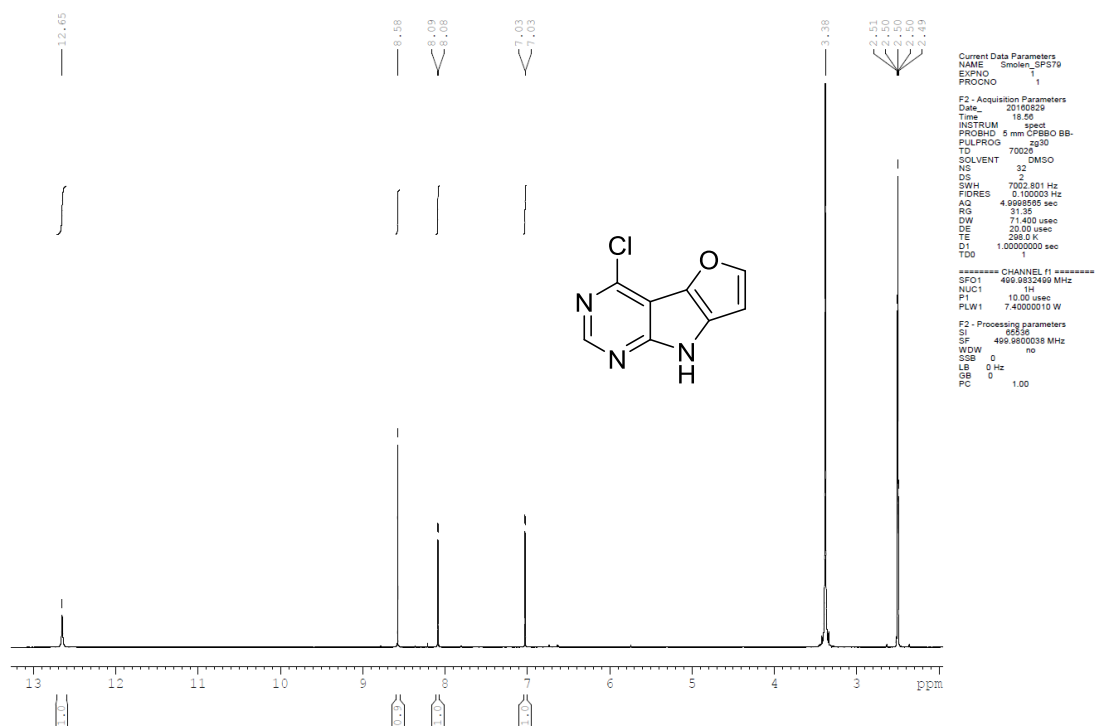
TOKARENKO ATH-434
 1H NMR in DMSO-d6
 14-02-16 RA



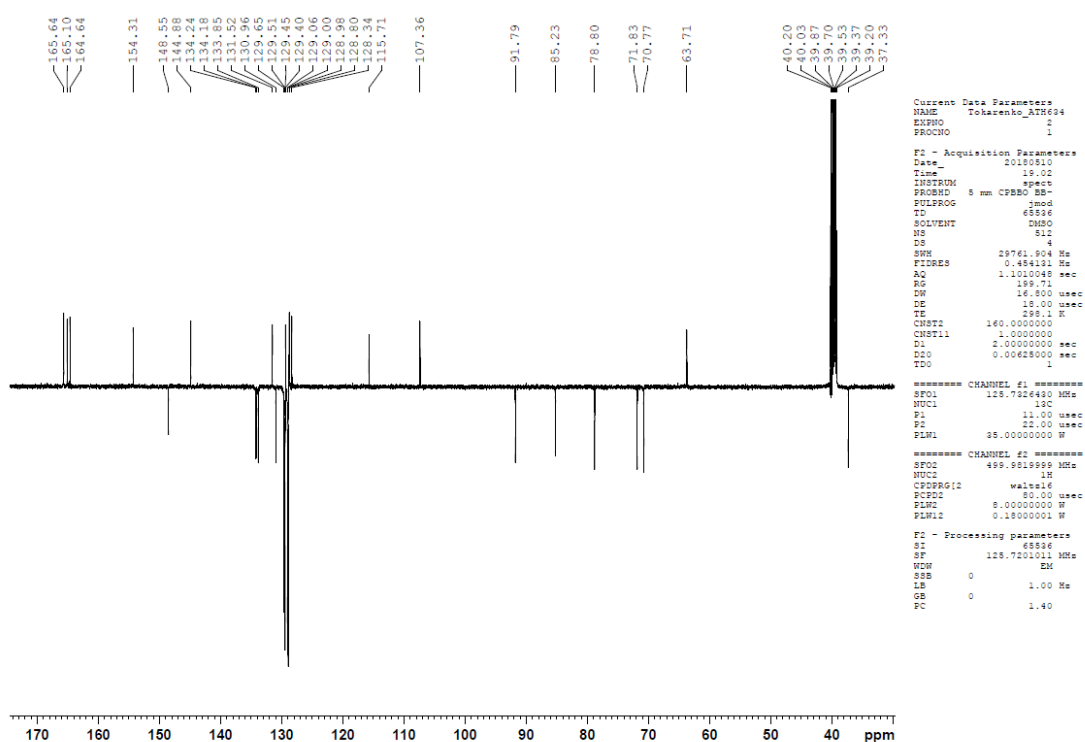
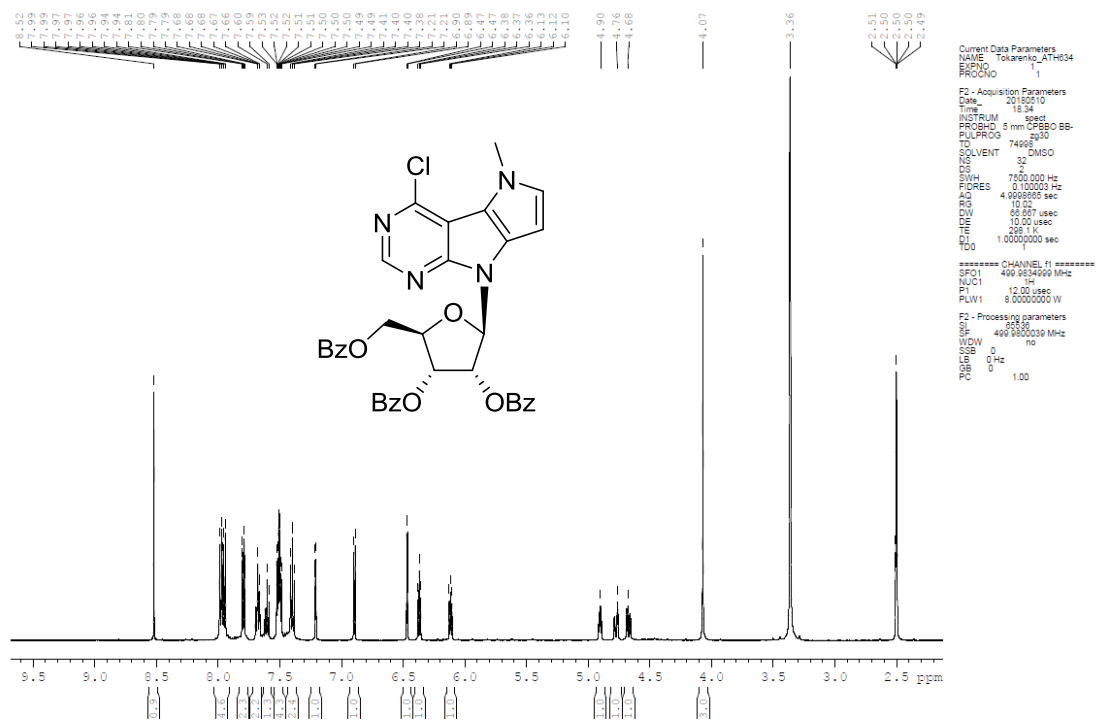
TOKARENKO ATH-434
 APT in DMSO-d6
 14-03-16 RA

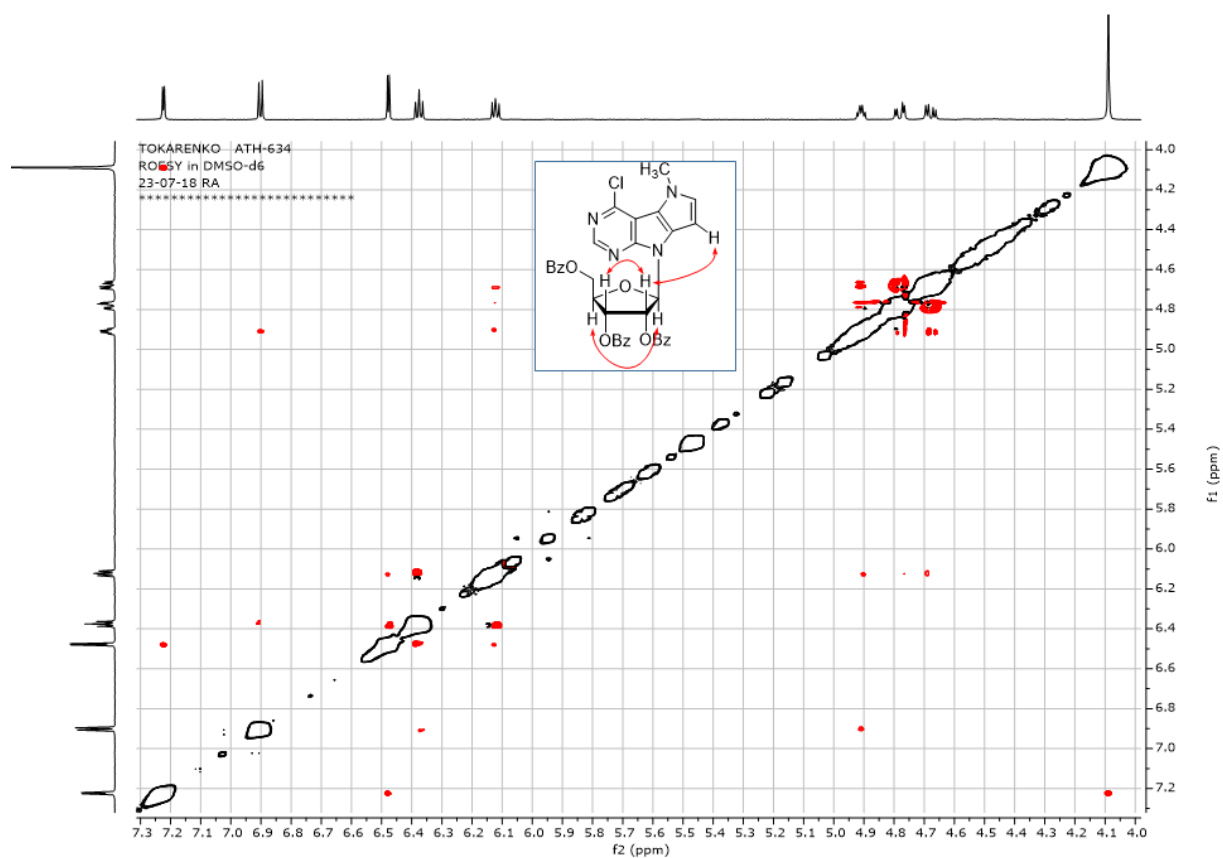


NMR spectra of compound **17**

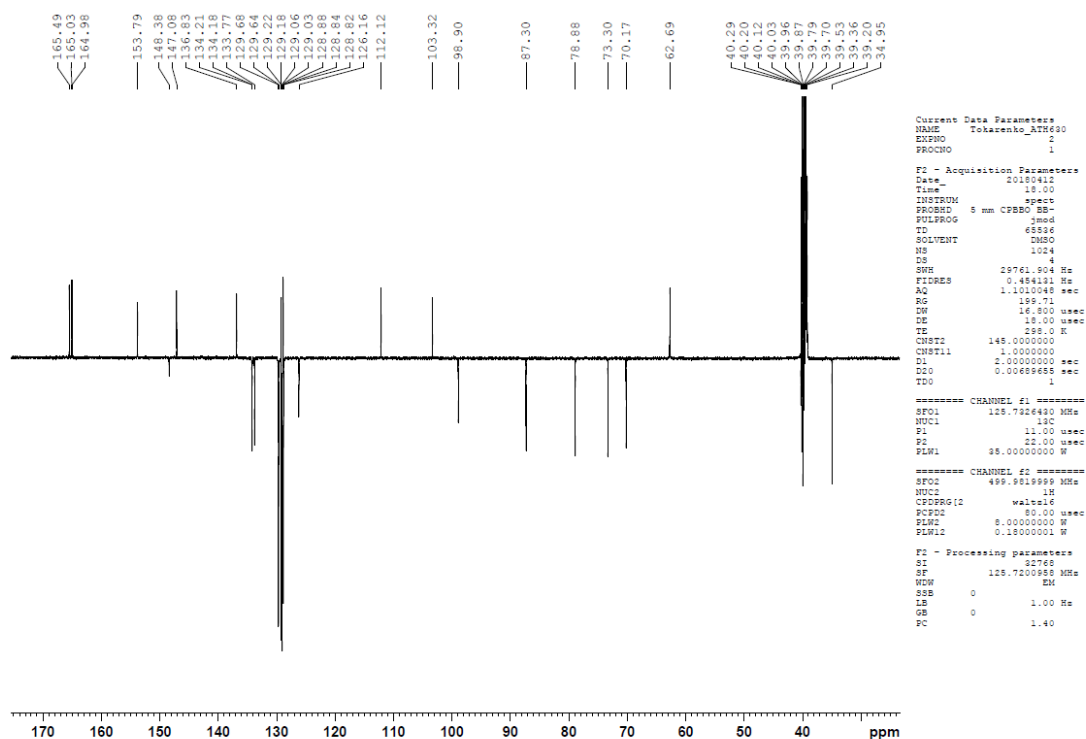
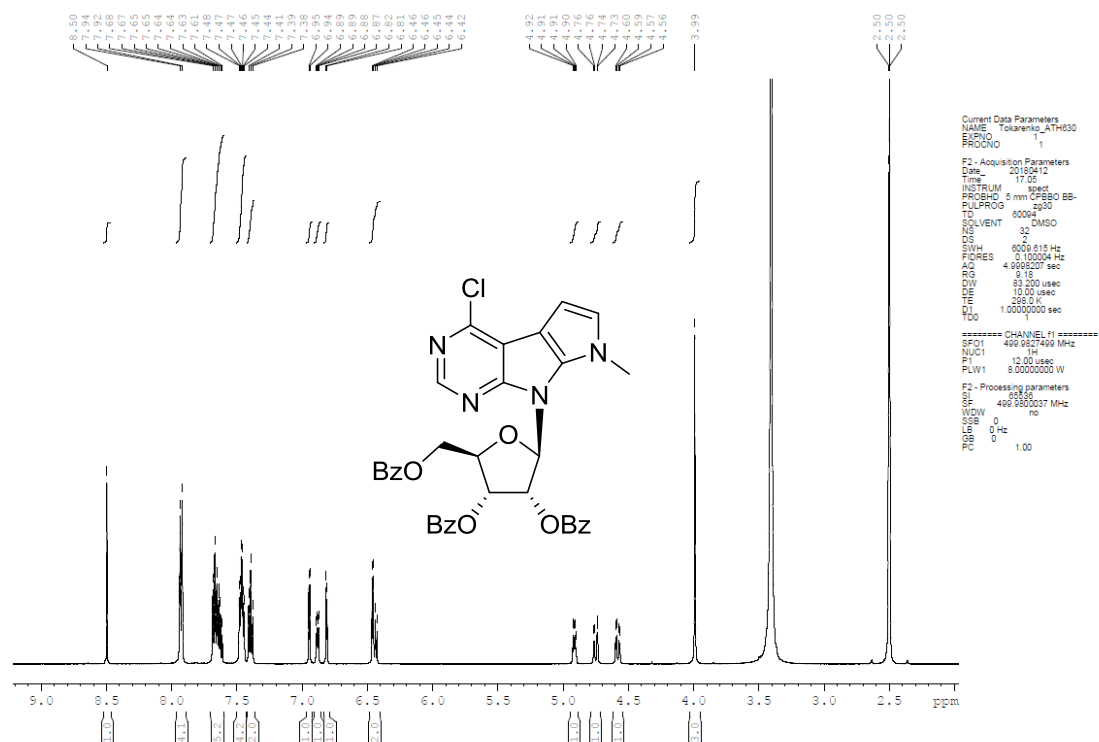


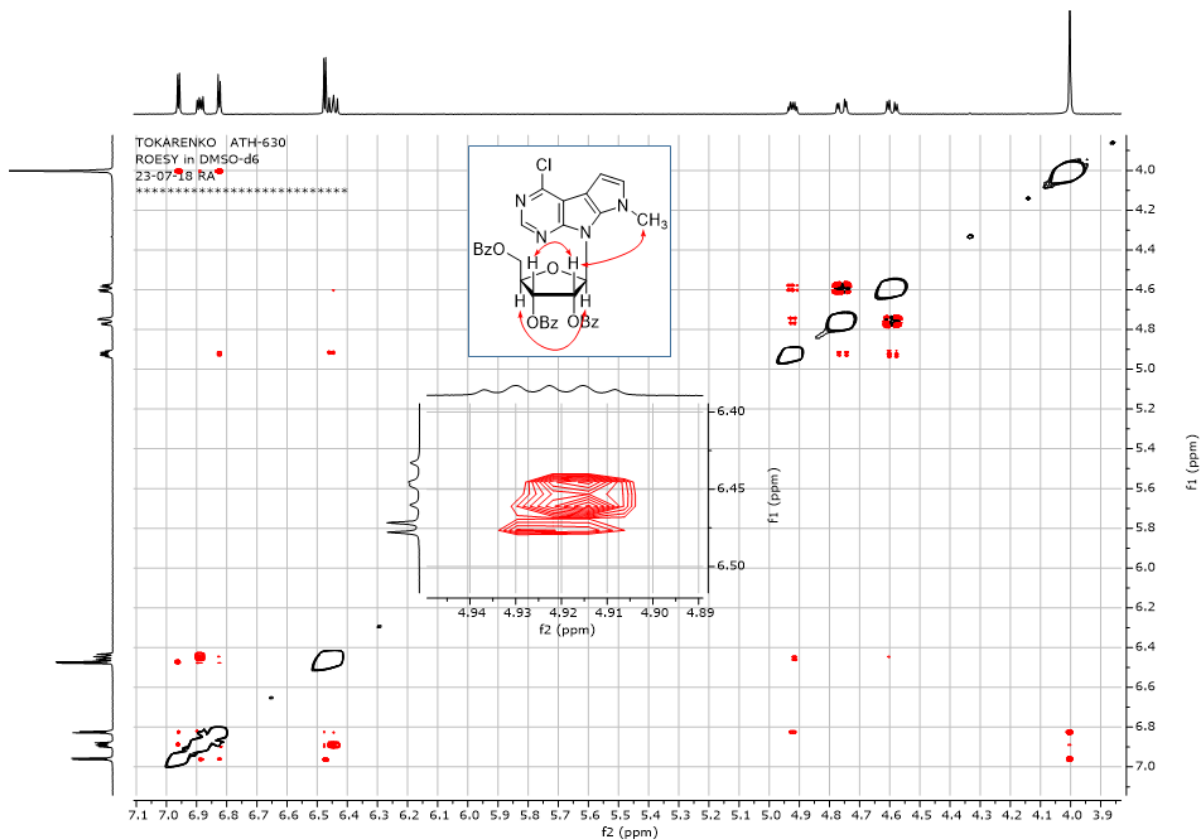
NMR spectra of compound **18**



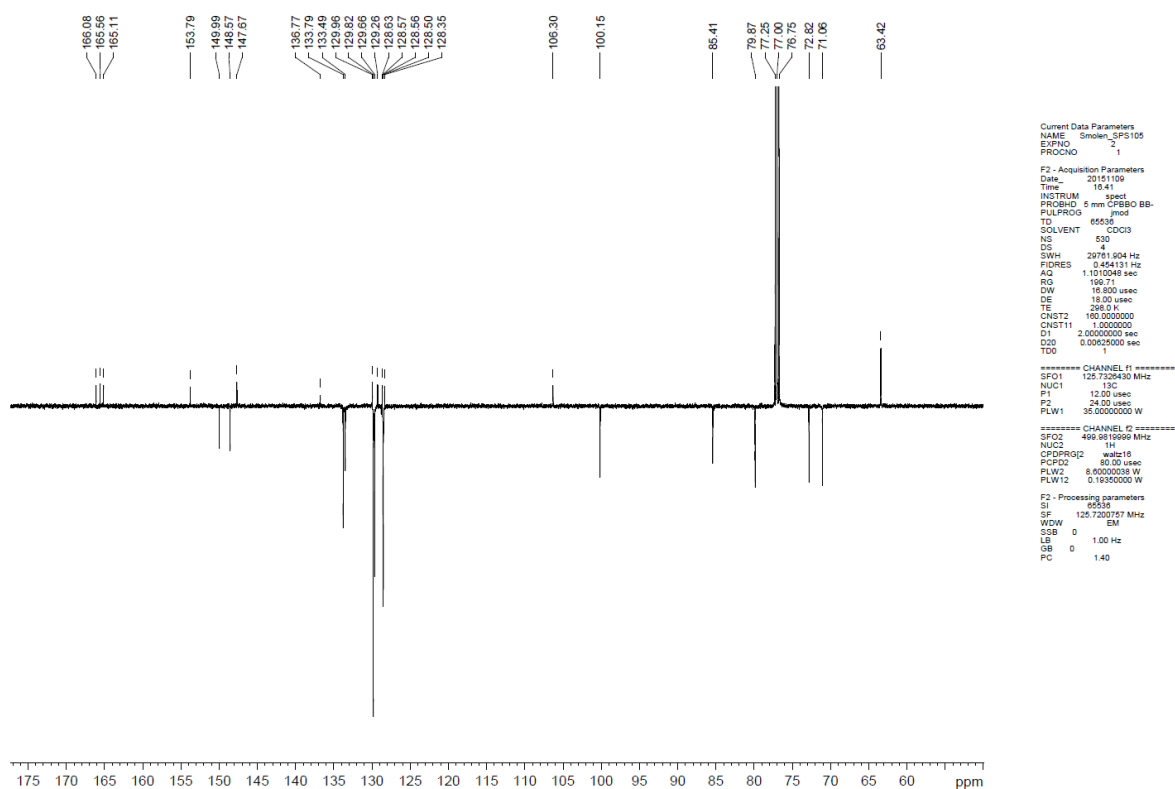
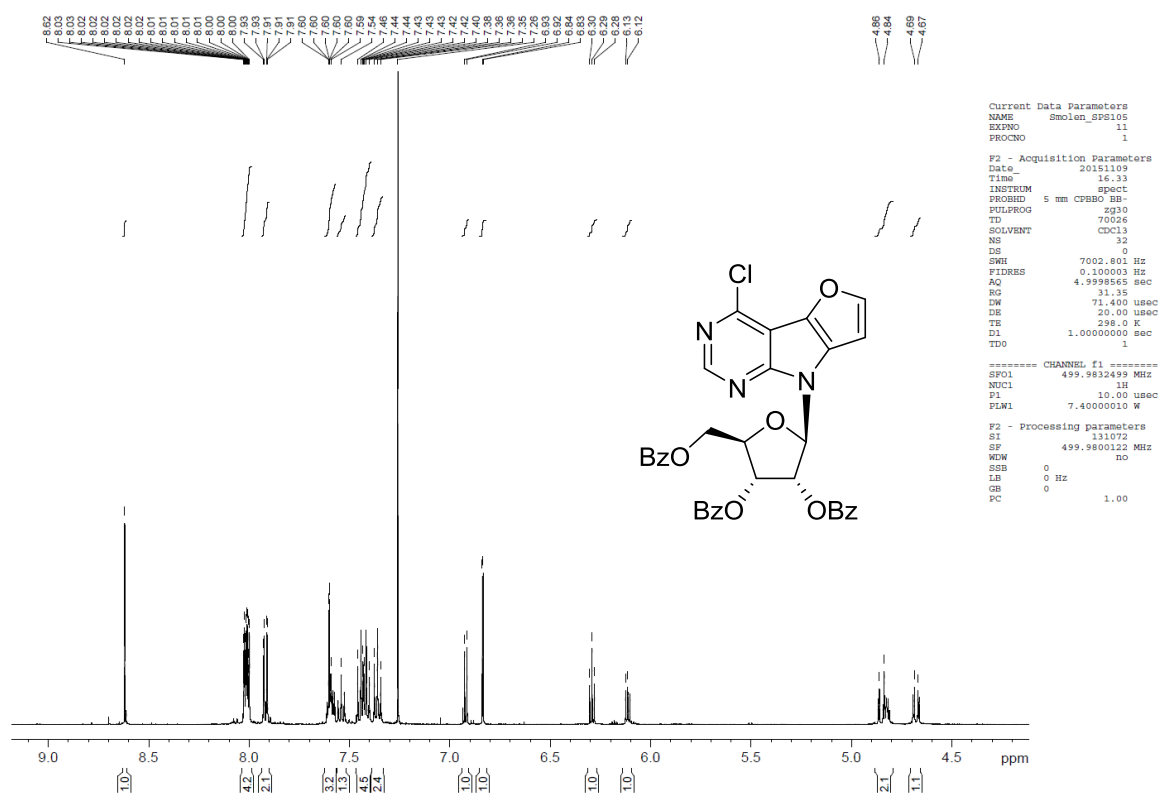


NMR spectra of compound **19**

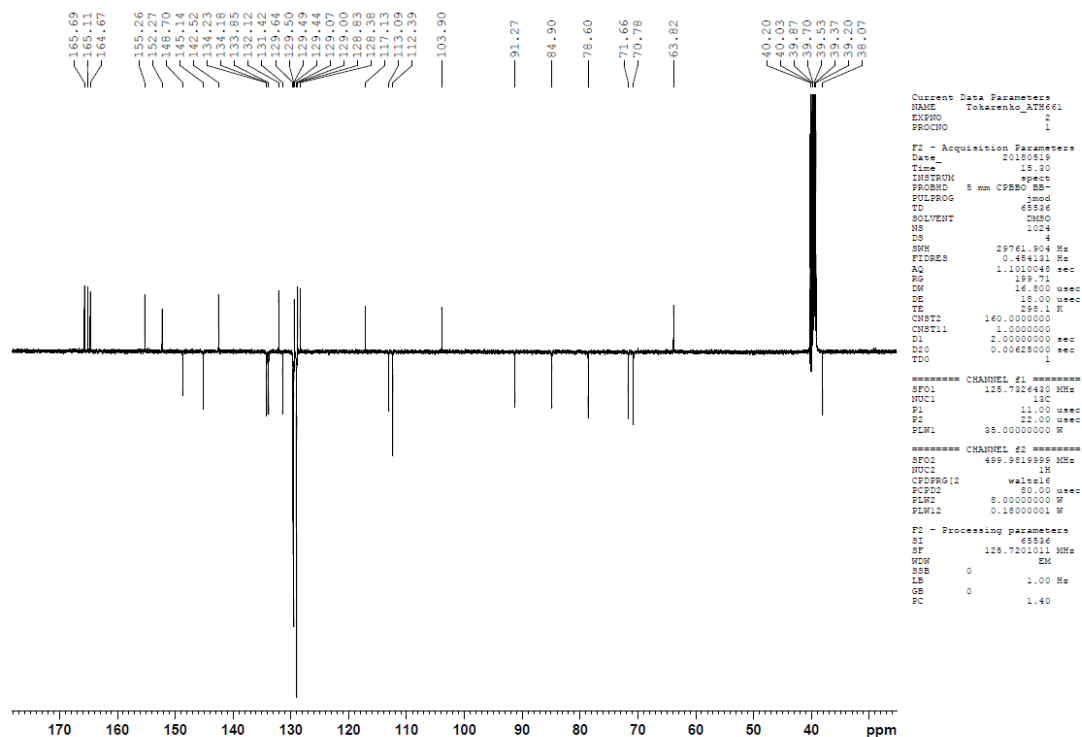




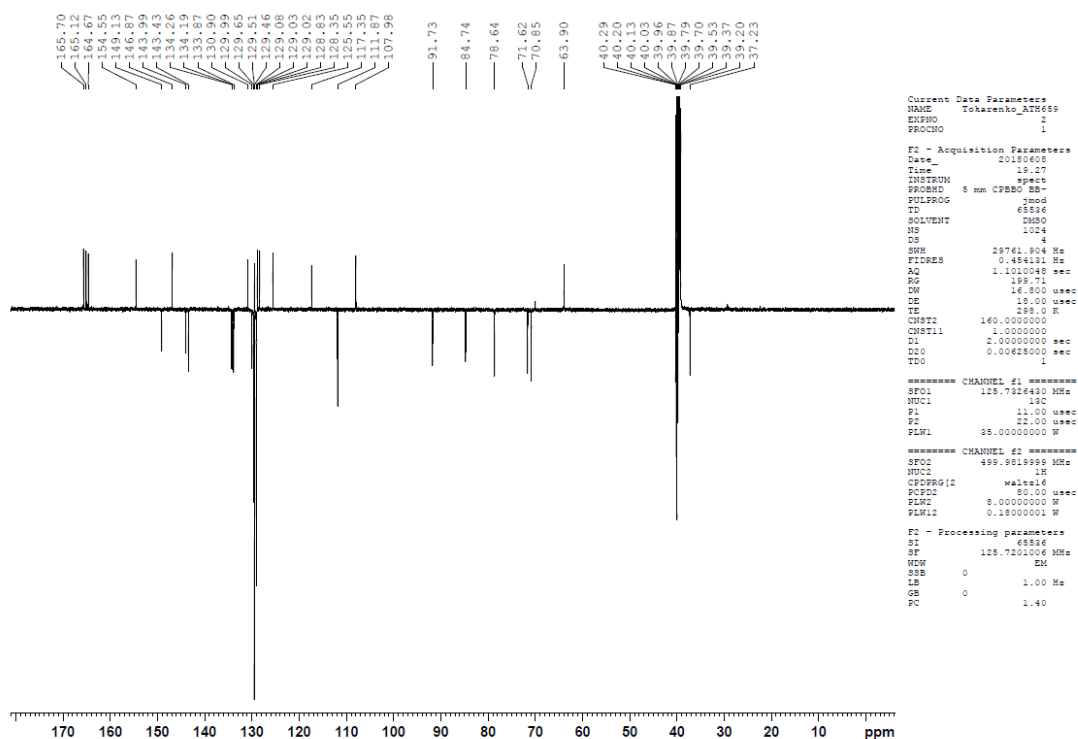
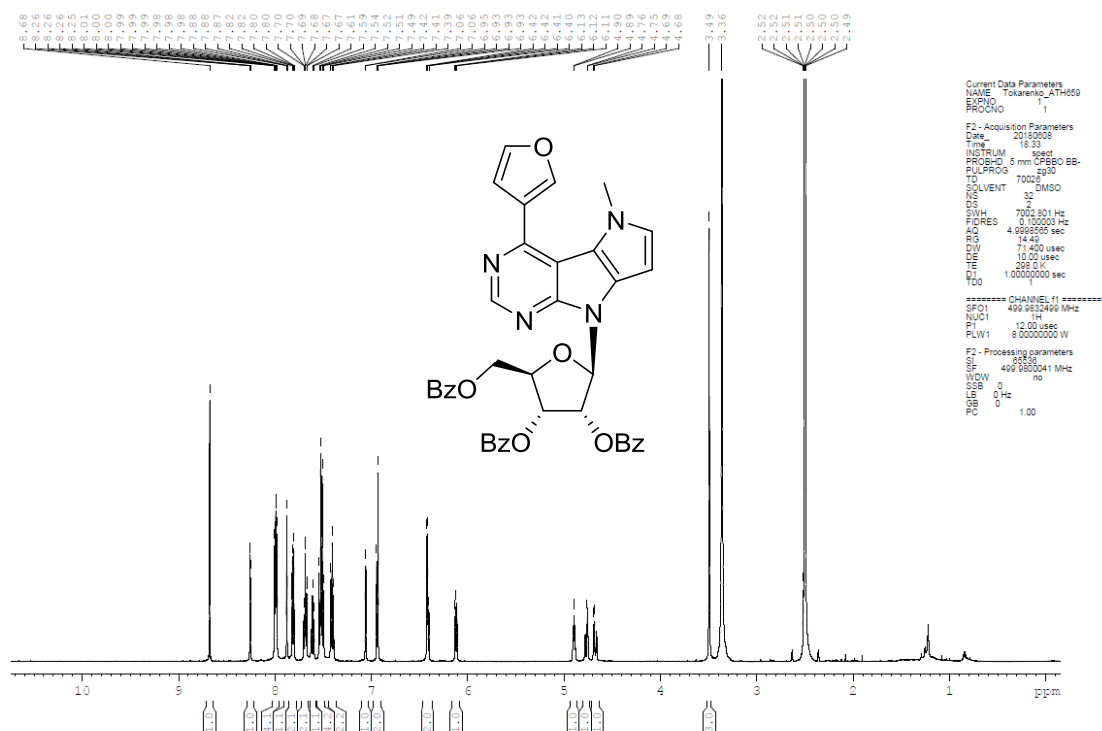
NMR spectra of compound 20



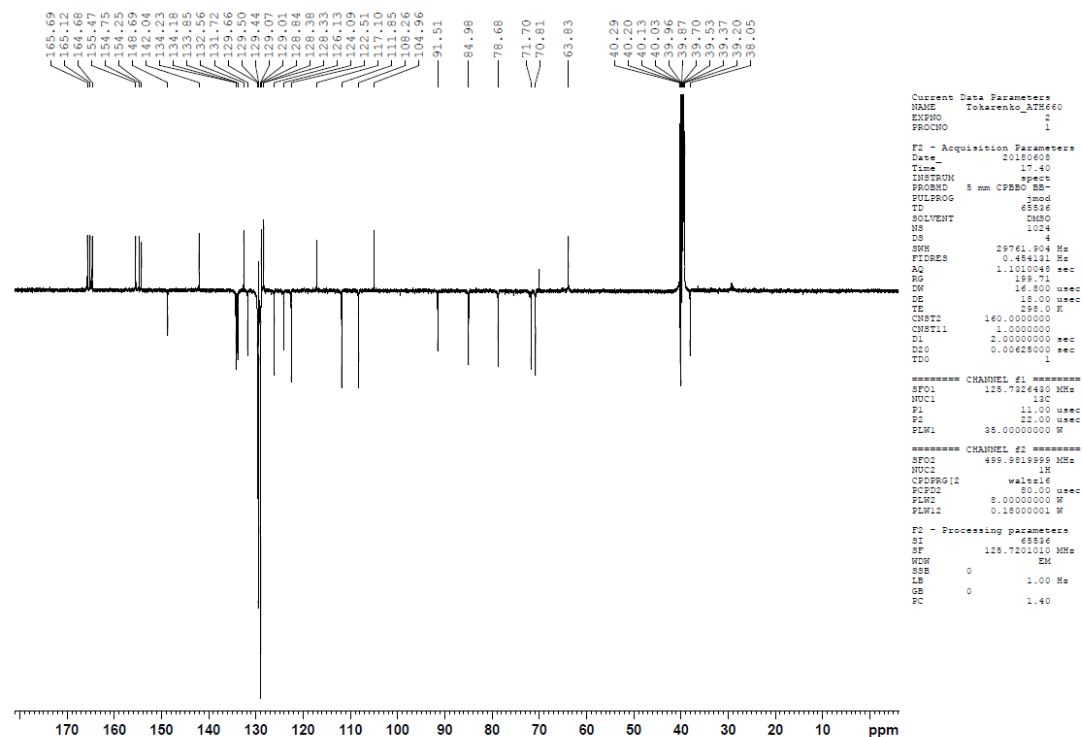
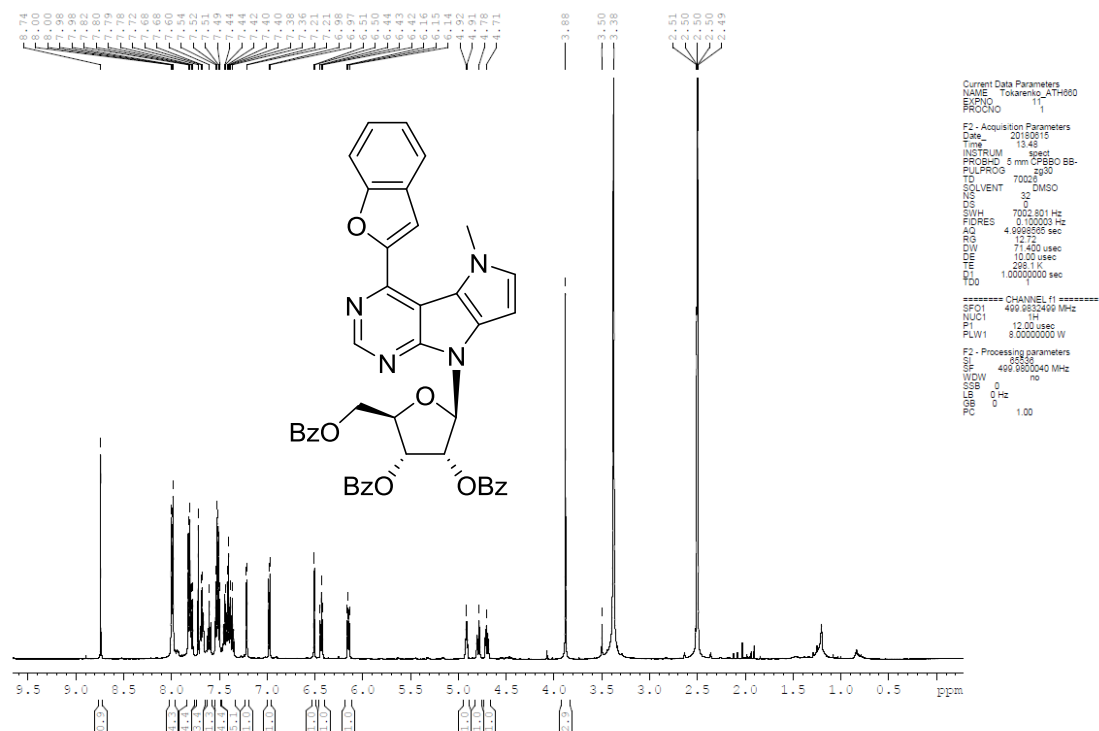
S21



NMR spectra of compound **21b**



S23

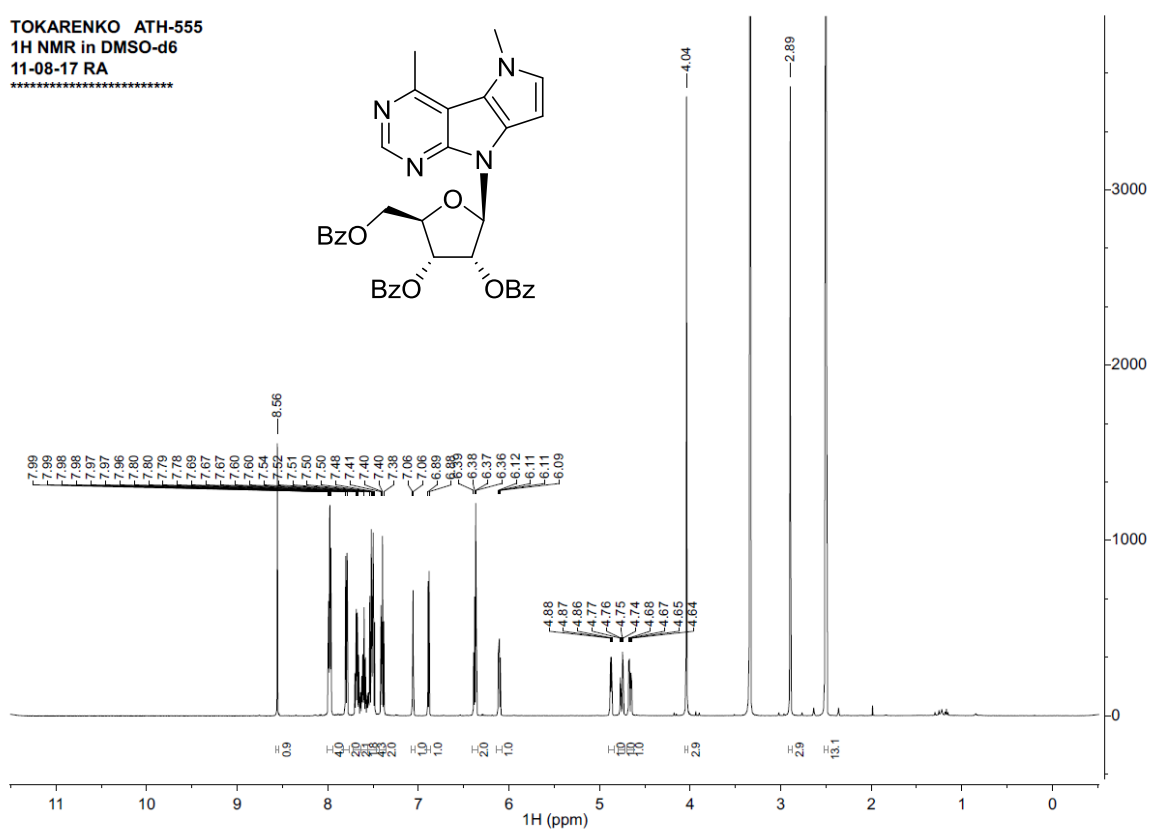


NMR spectra of compound **21d**

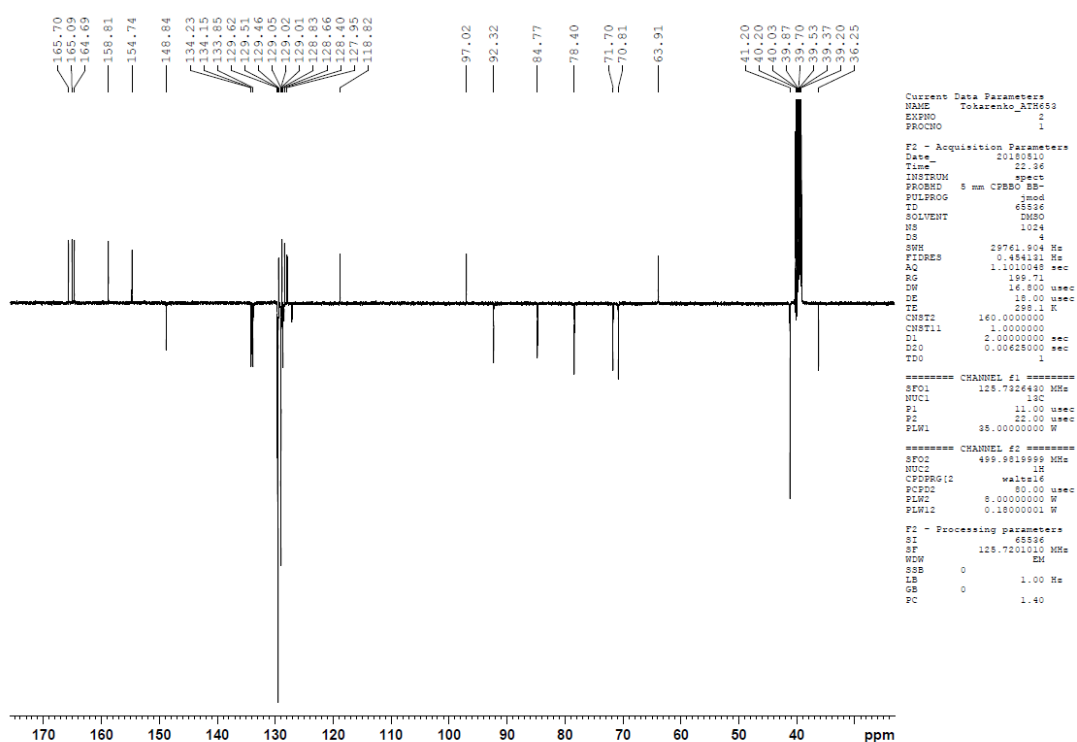
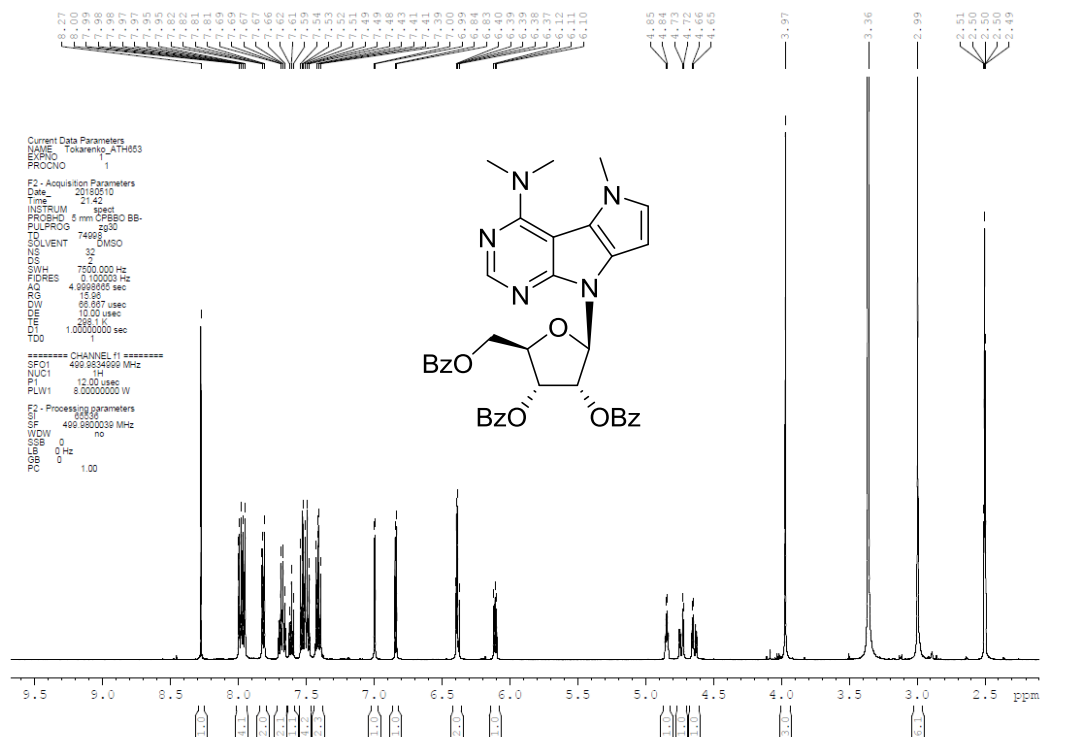
TOKARENKO ATH-555

¹H NMR in DMSO-d₆

11-08-17 RA

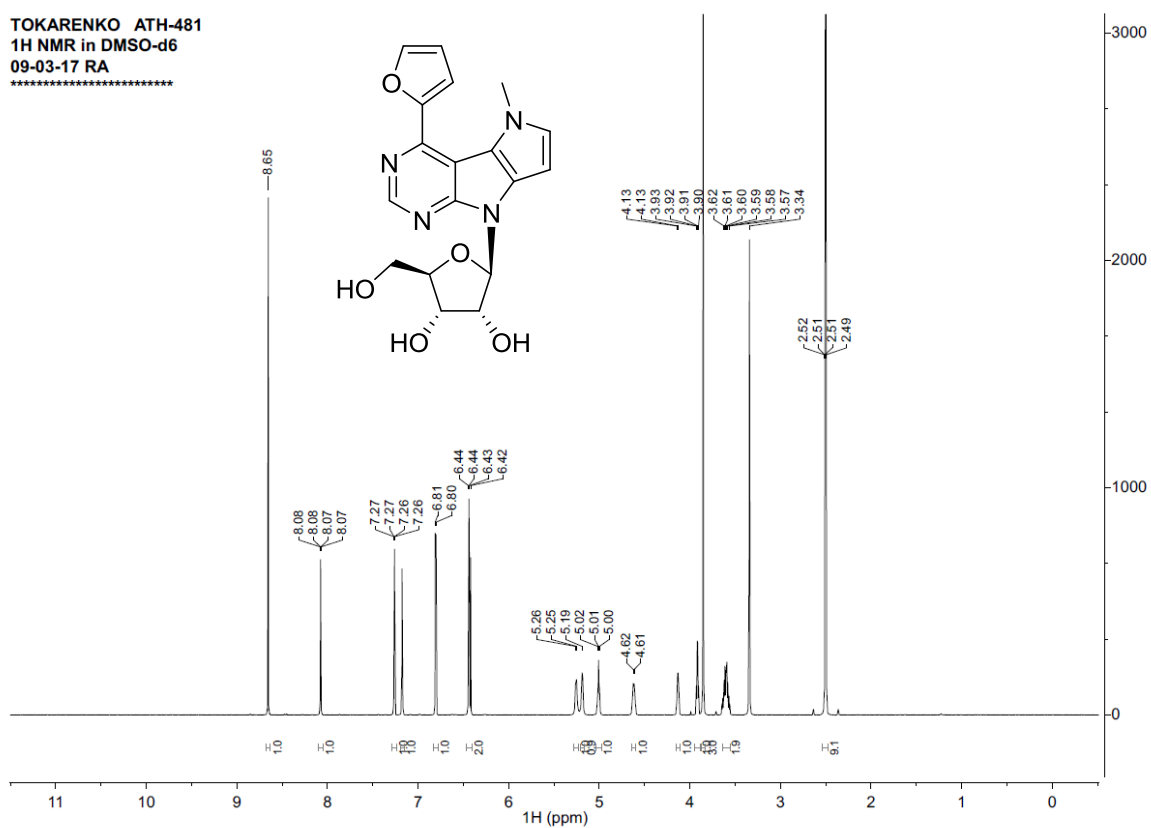


NMR spectra of compound **21e**

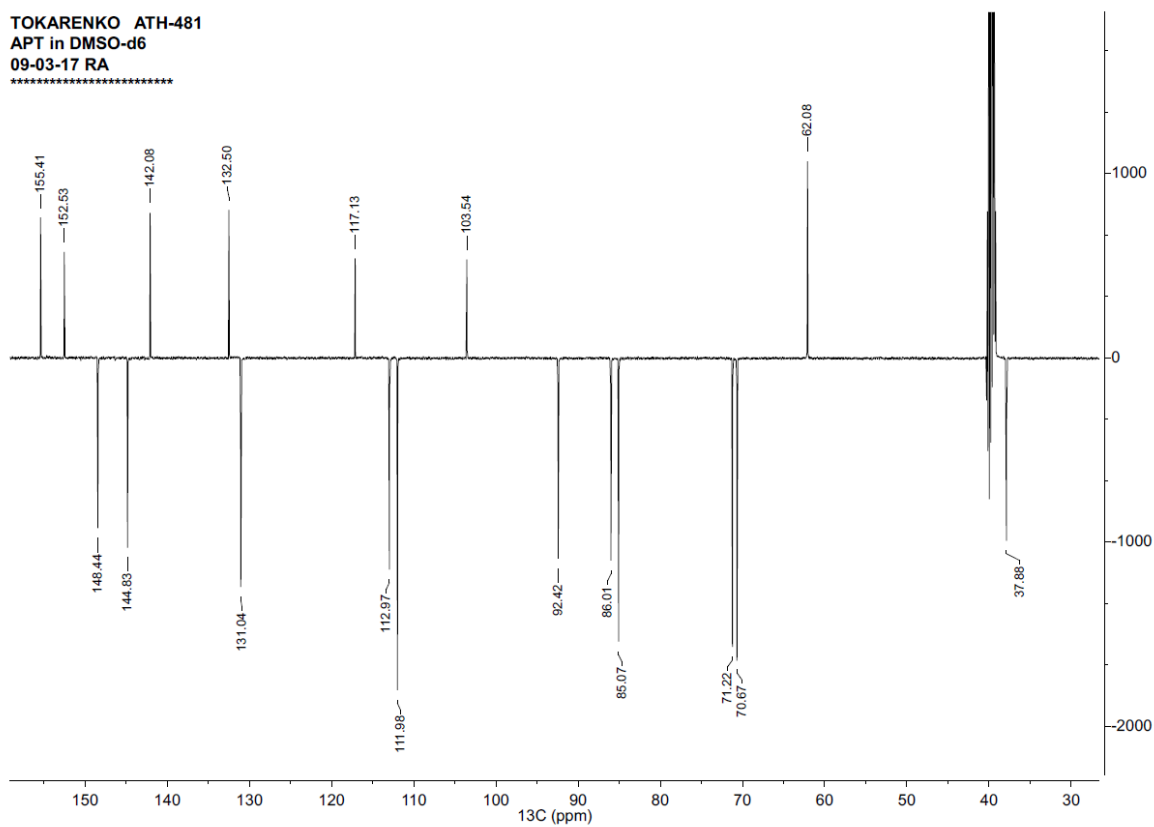


NMR spectra of compound **22a**

TOKARENKO ATH-481
 1H NMR in DMSO-d6
 09-03-17 RA

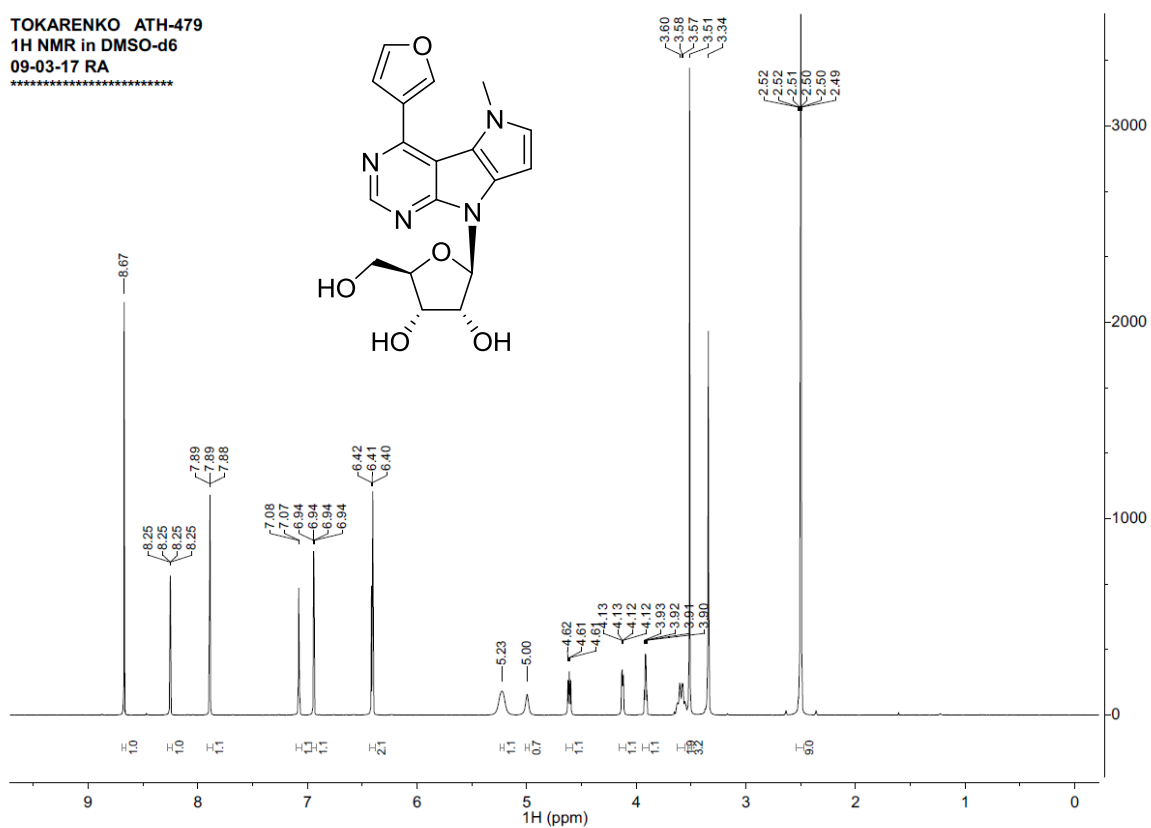


TOKARENKO ATH-481
 APT in DMSO-d6
 09-03-17 RA

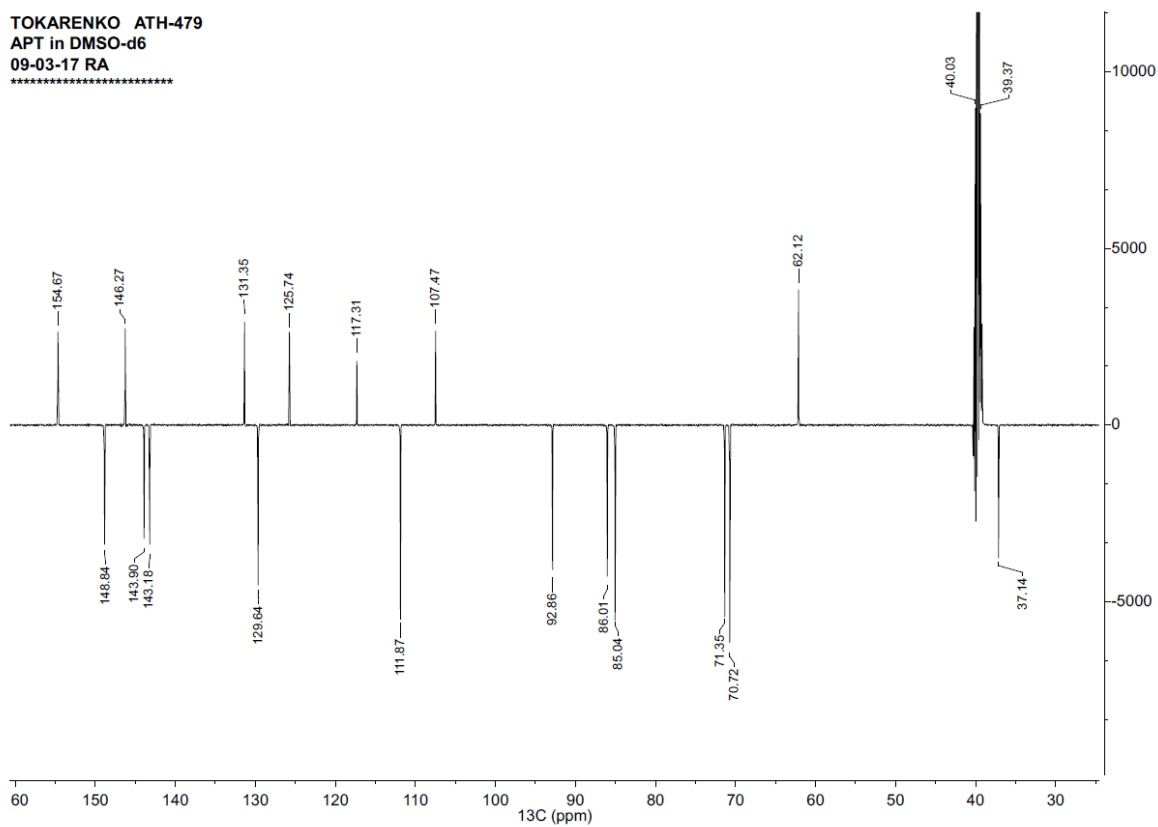


NMR spectra of compound **22b**

TOKARENKO ATH-479
 1H NMR in DMSO-d6
 09-03-17 RA

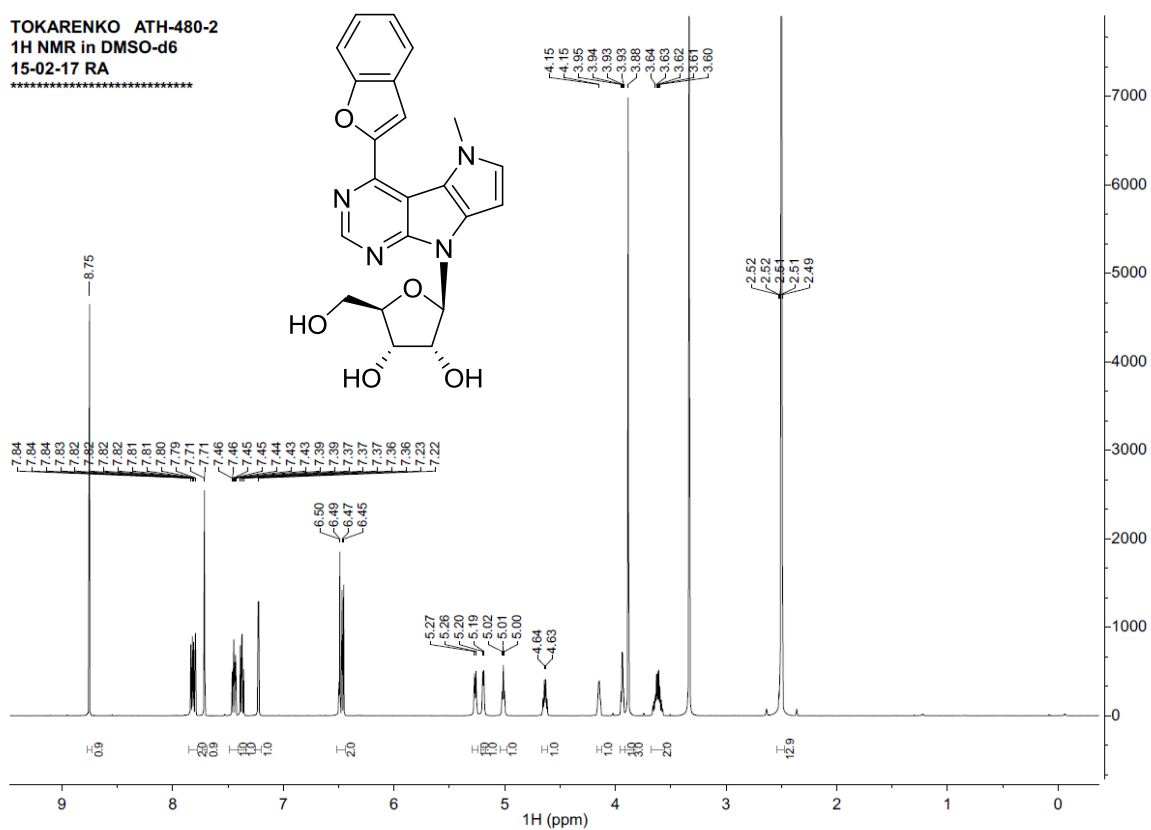


TOKARENKO ATH-479
 APT in DMSO-d6
 09-03-17 RA

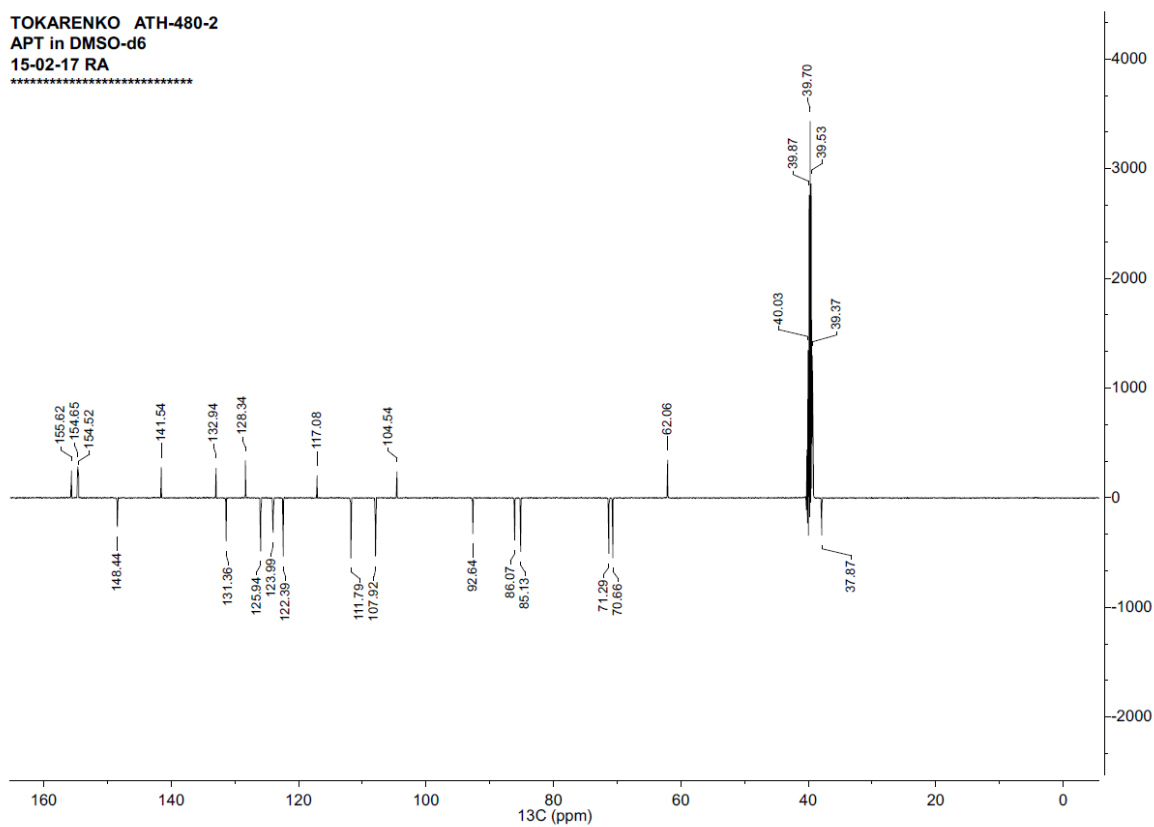


NMR spectra of compound **22c**

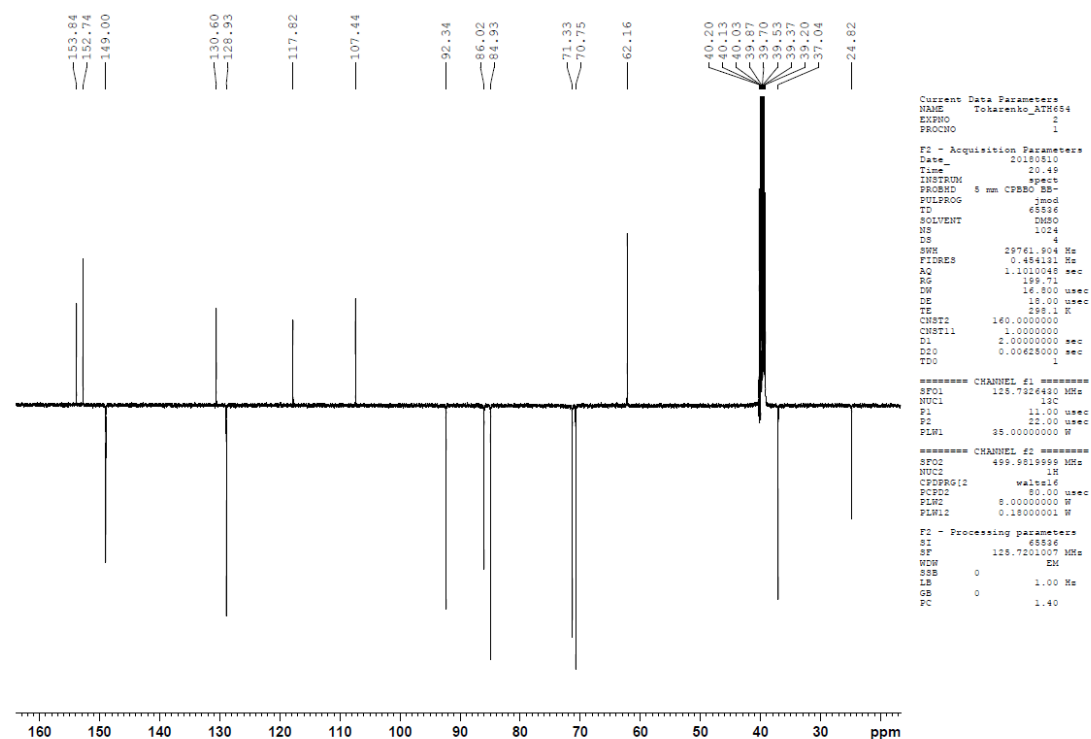
TOKARENKO ATH-480-2
1H NMR in DMSO-d6
15-02-17 RA



TOKARENKO ATH-480-2
APT in DMSO-d6
15-02-17 RA



S29

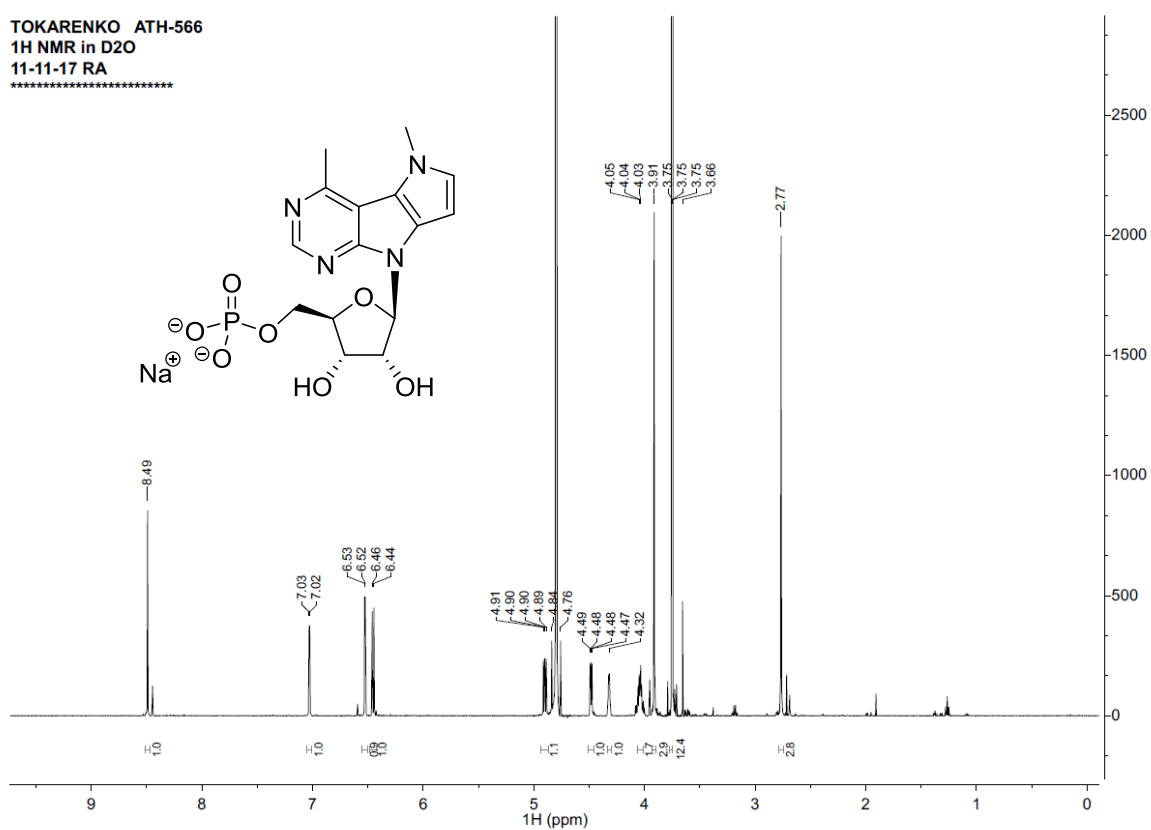


NMR spectra of compound **22d-MP**

TOKARENKO ATH-566

¹H NMR in D₂O

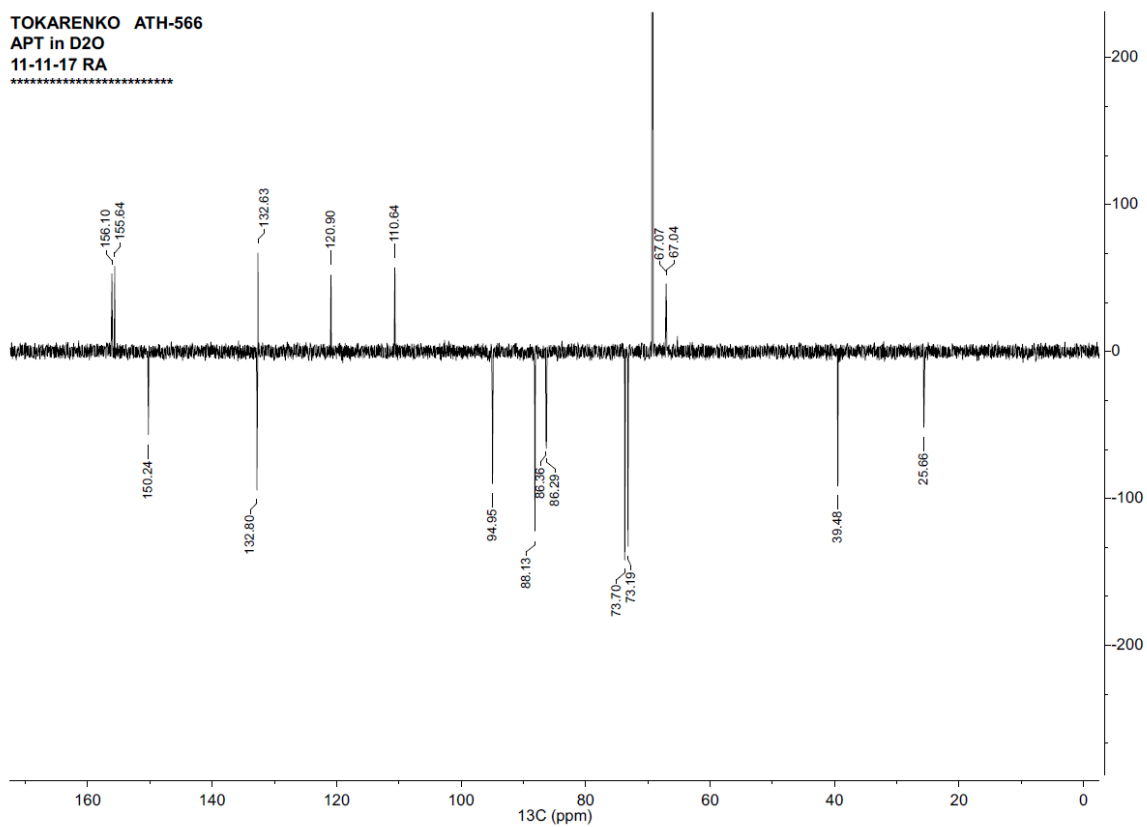
11-11-17 RA



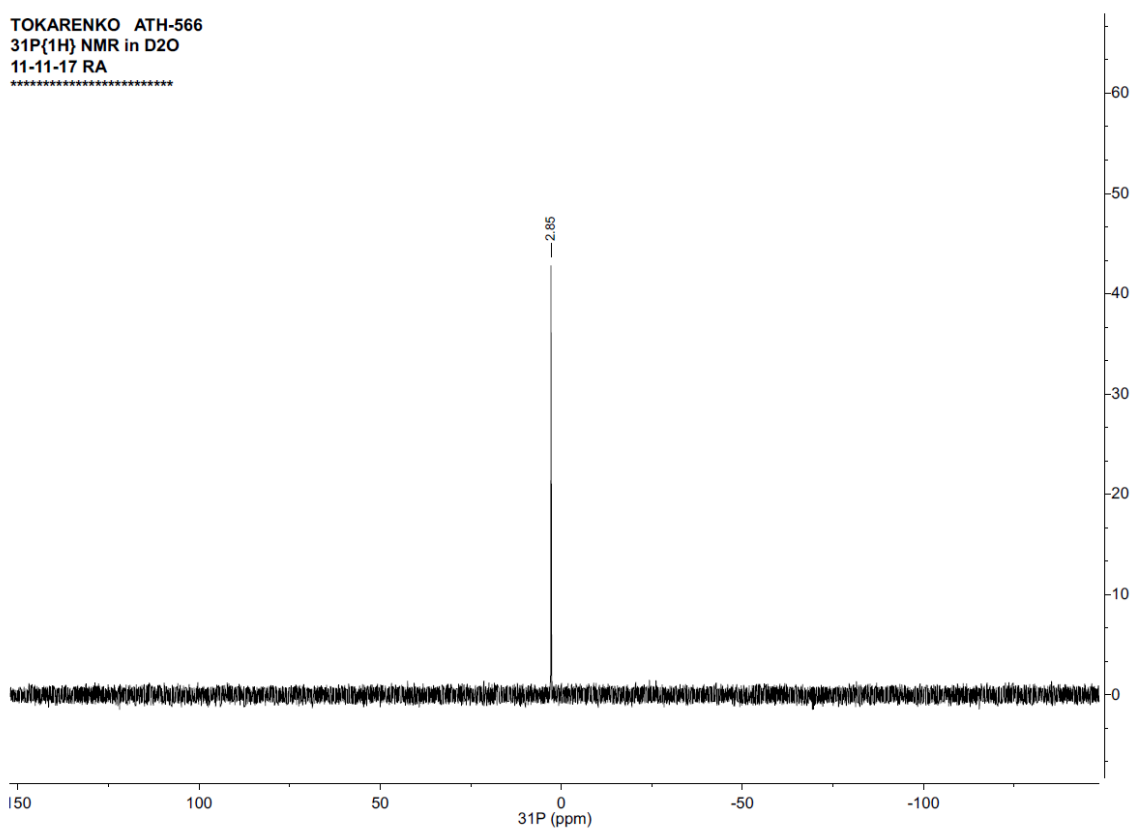
TOKARENKO ATH-566

APT in D₂O

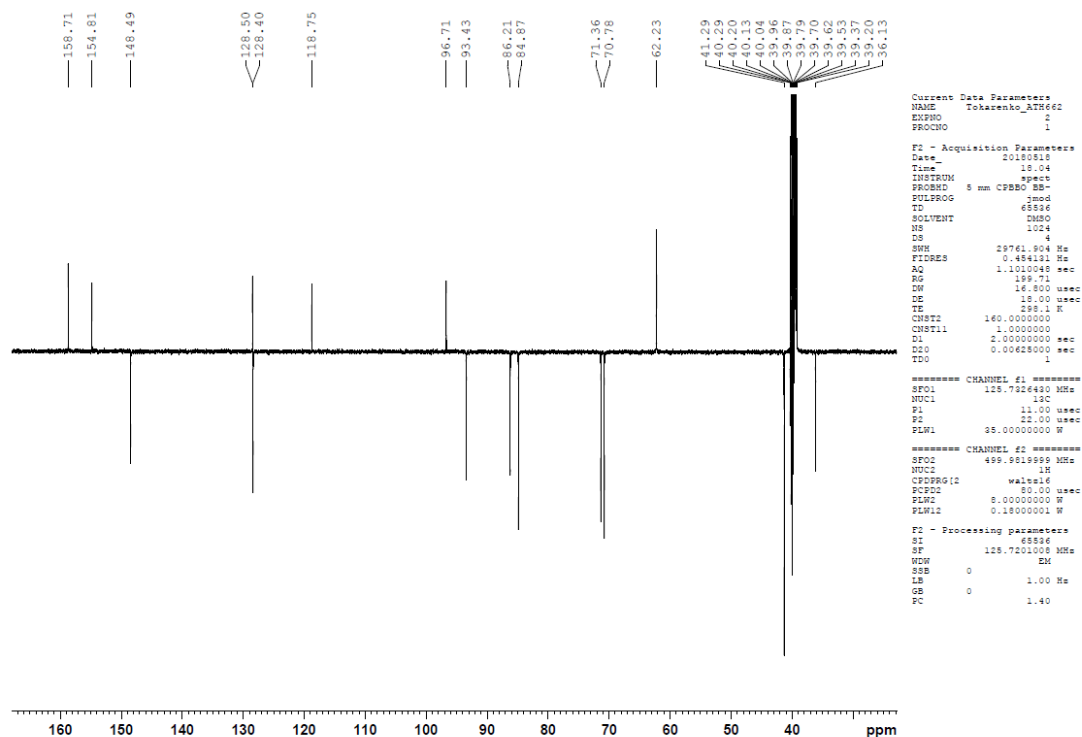
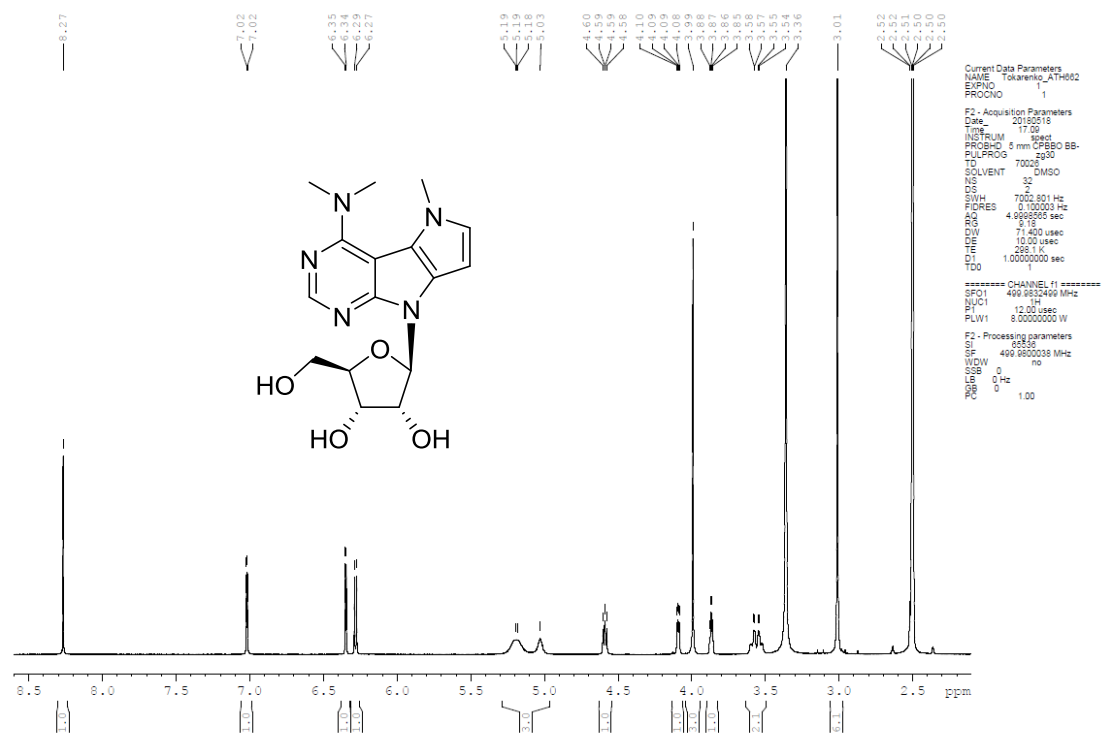
11-11-17 RA



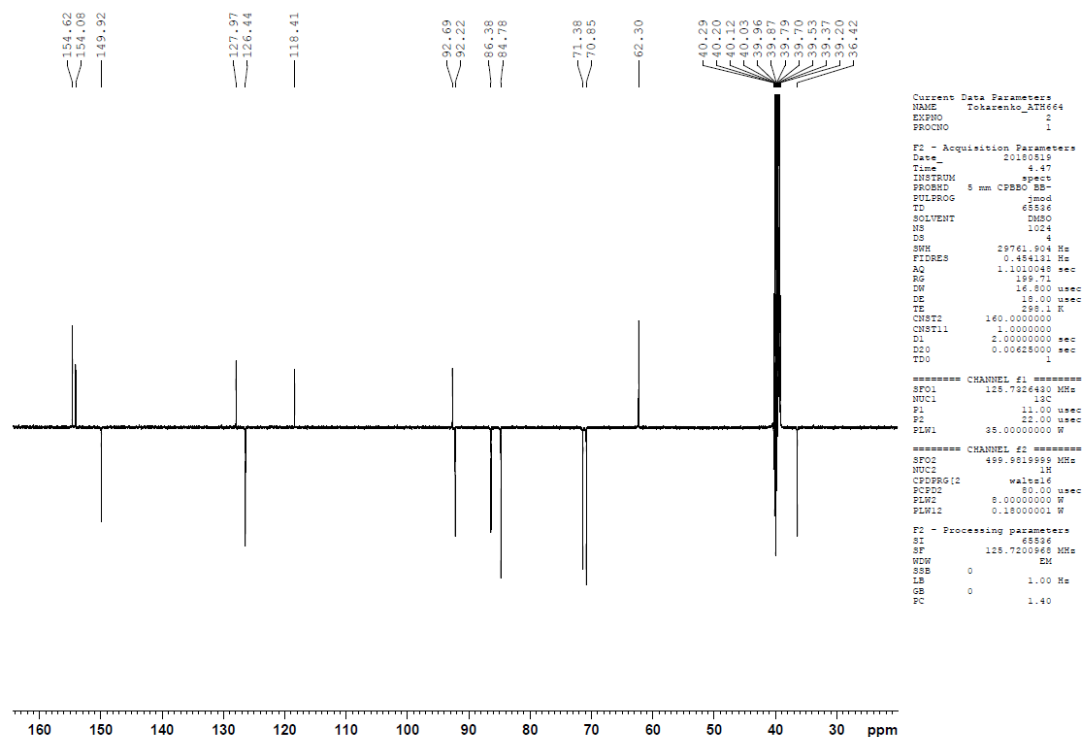
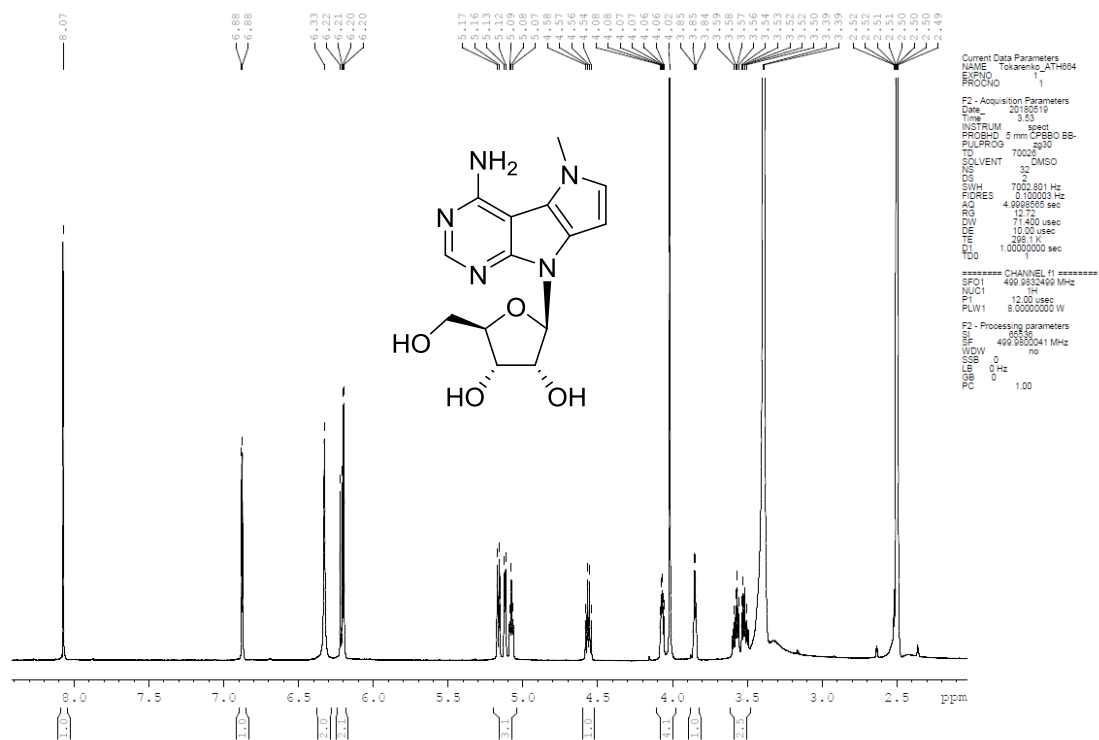
TOKARENKO ATH-566
31P{1H} NMR in D2O
11-11-17 RA



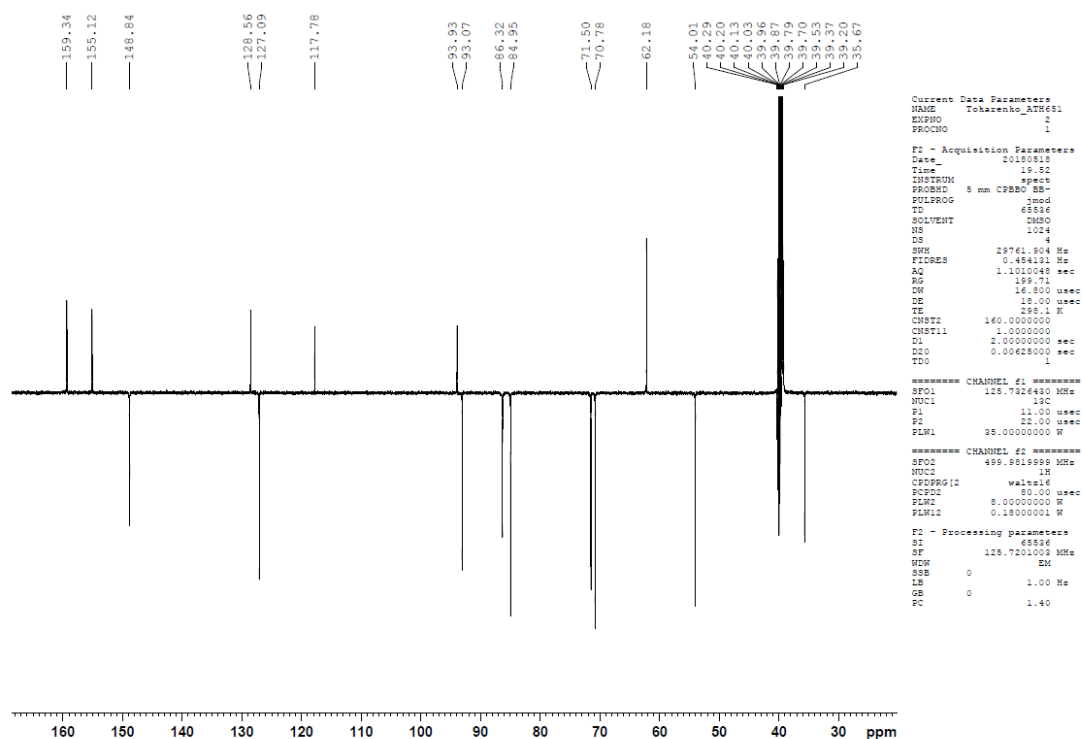
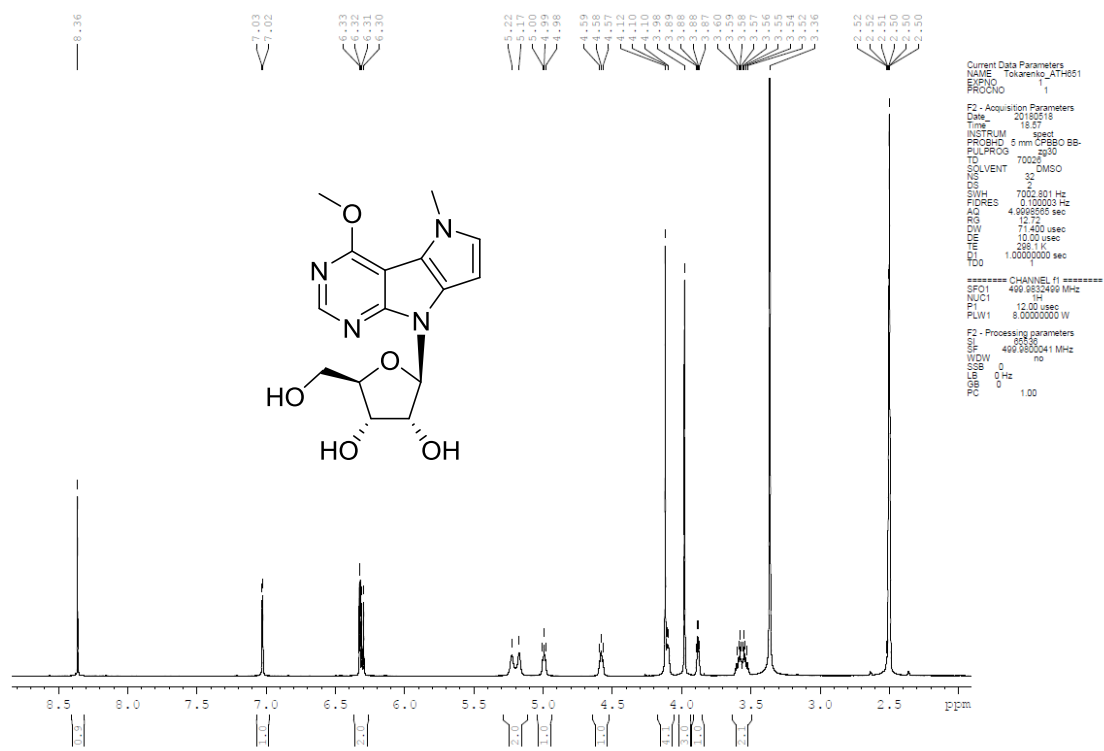
NMR spectra of compound **22e**



NMR spectra of compound **22f**

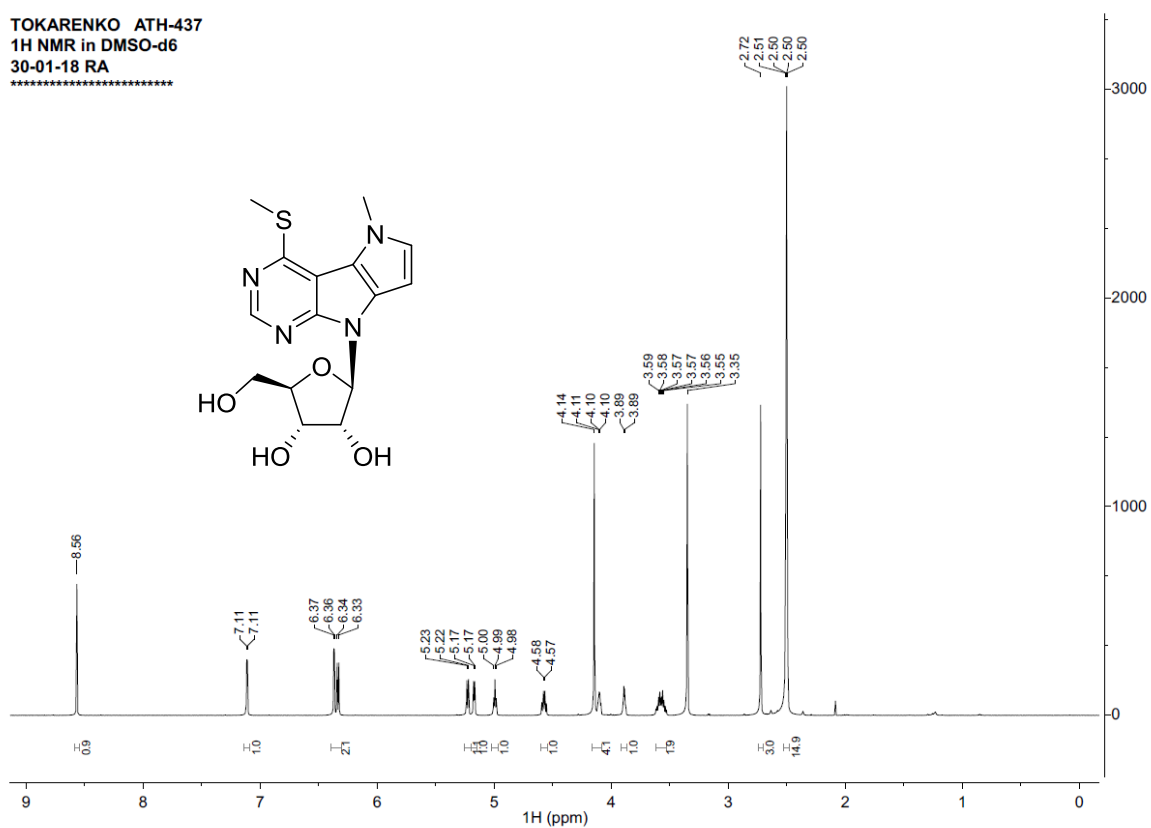


NMR spectra of compound **22g**

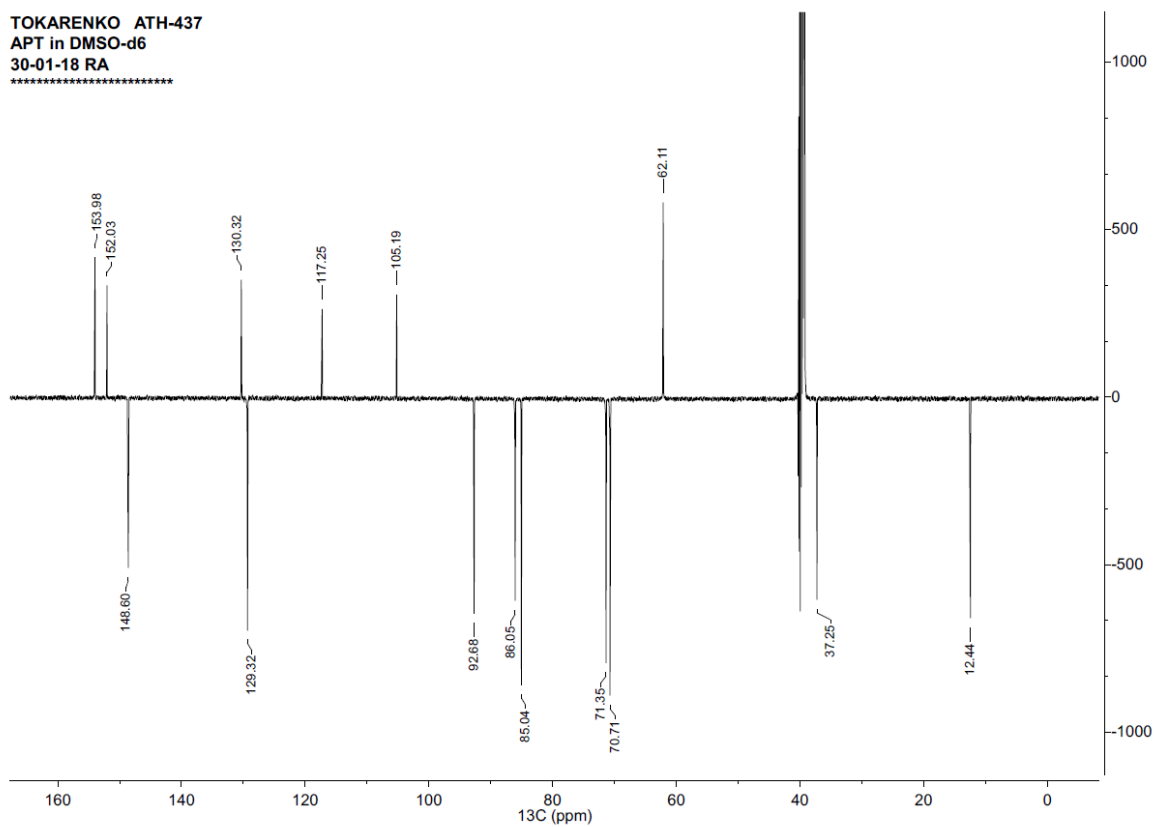


NMR spectra of compound **22h**

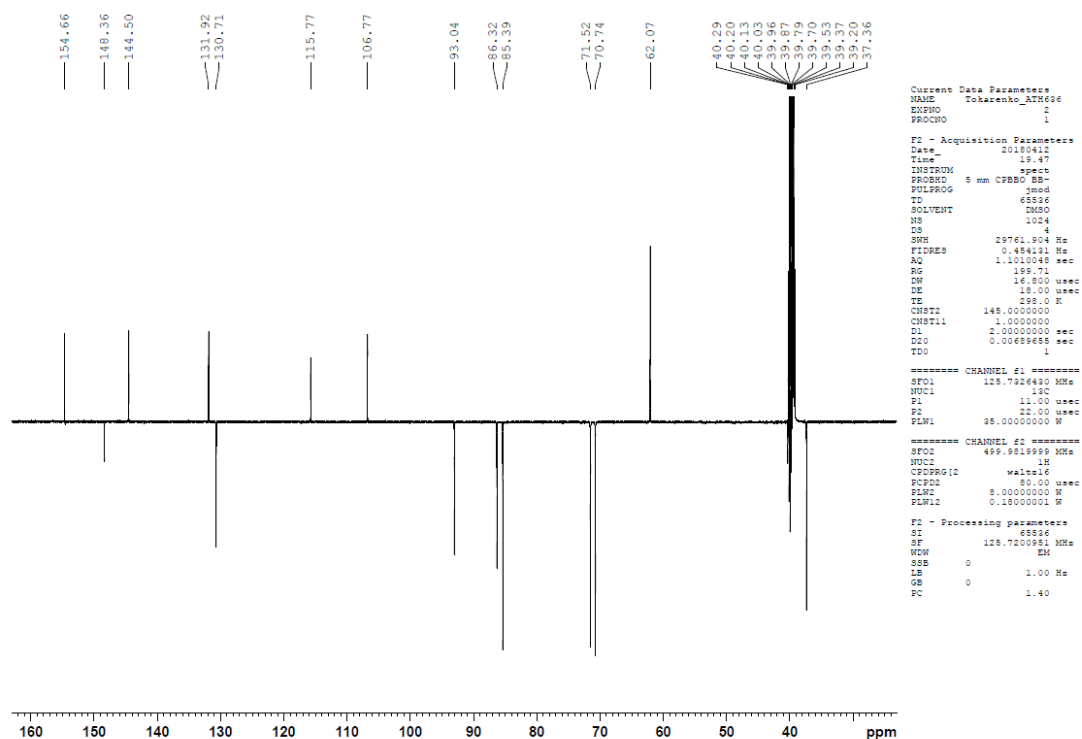
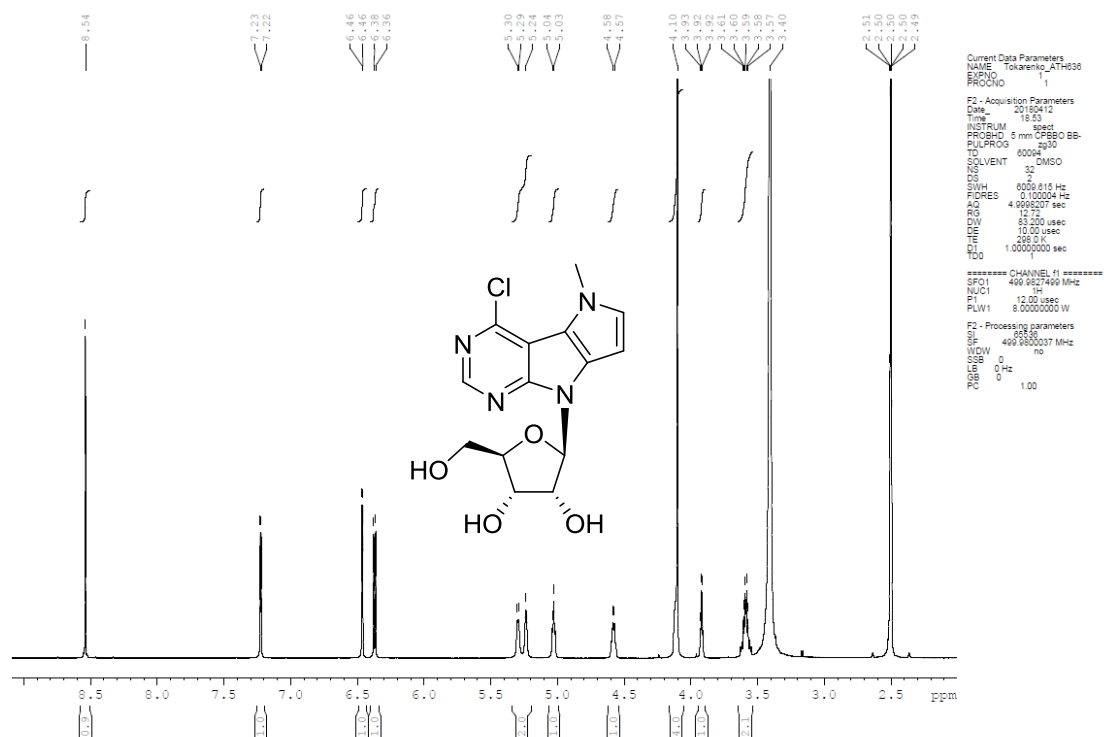
TOKARENKO ATH-437
 1H NMR in DMSO-d6
 30-01-18 RA



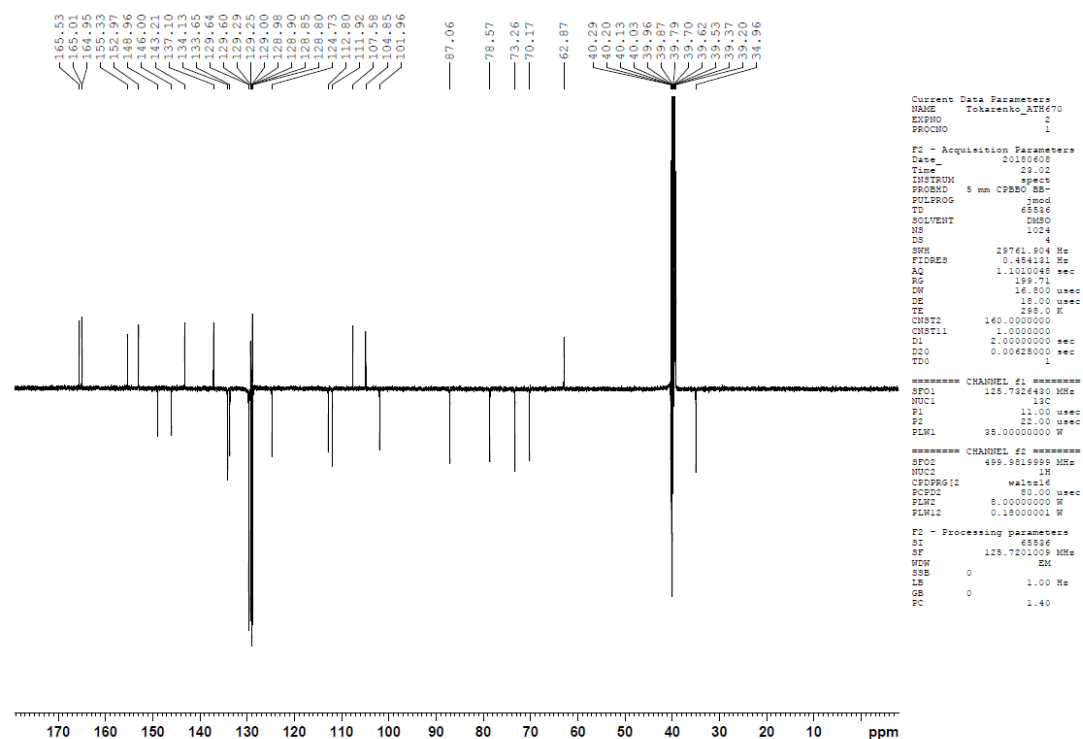
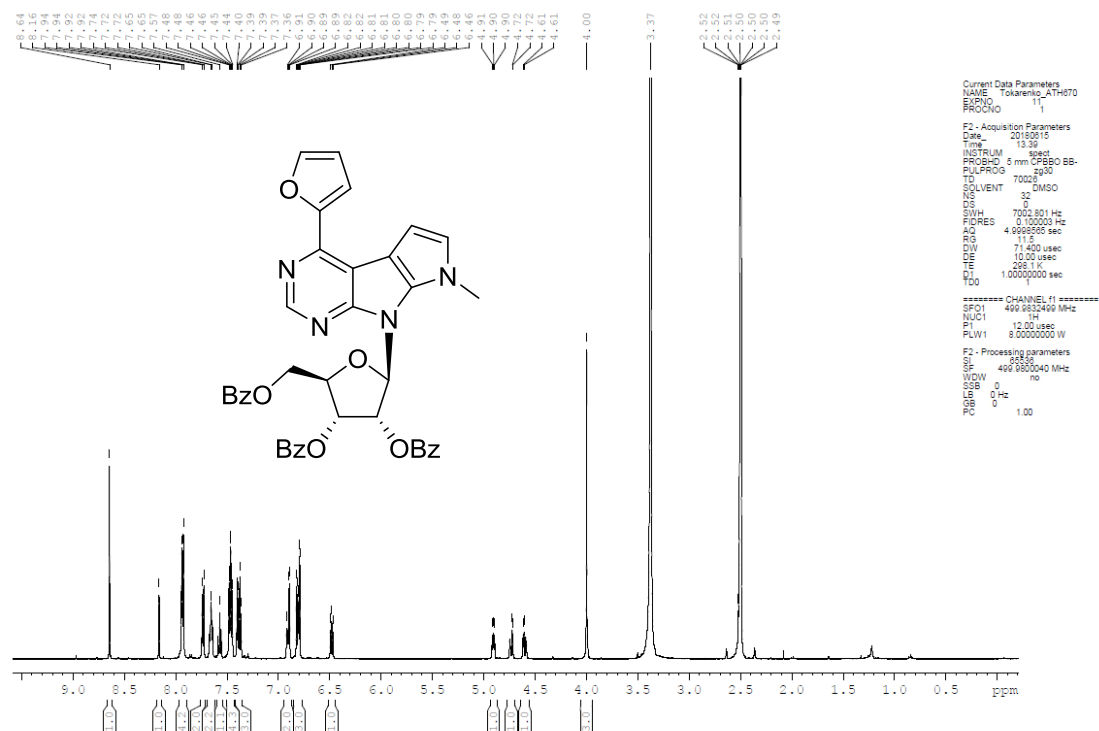
TOKARENKO ATH-437
 APT in DMSO-d6
 30-01-18 RA



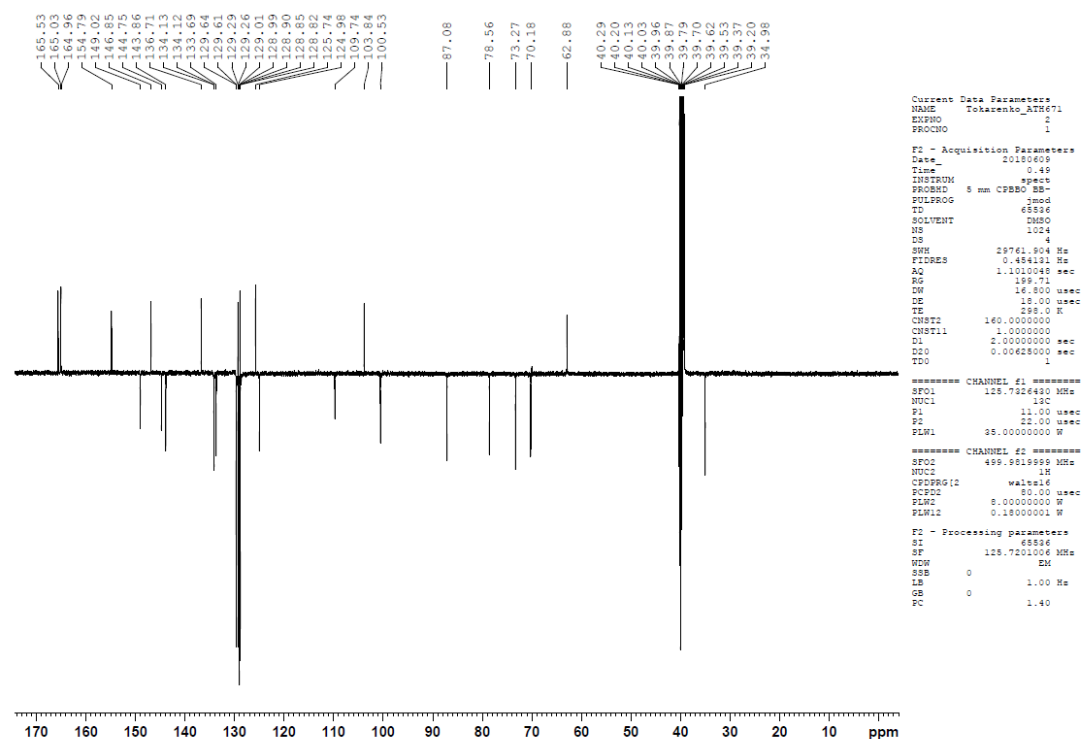
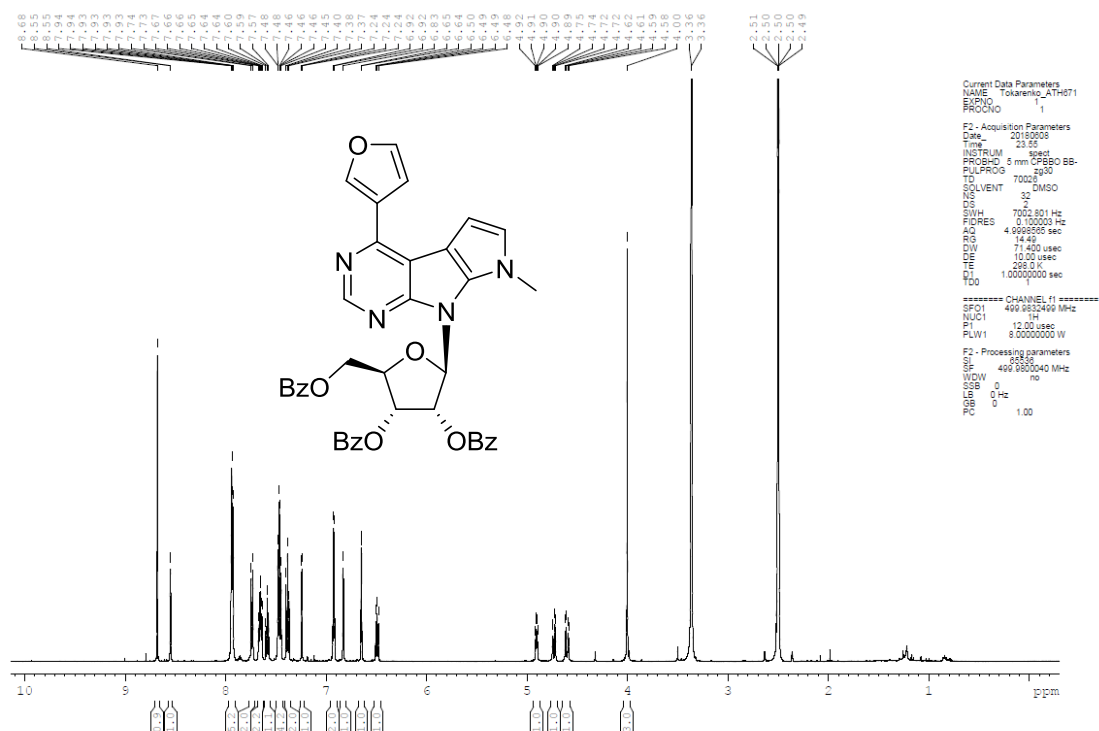
NMR spectra of compound **22i**



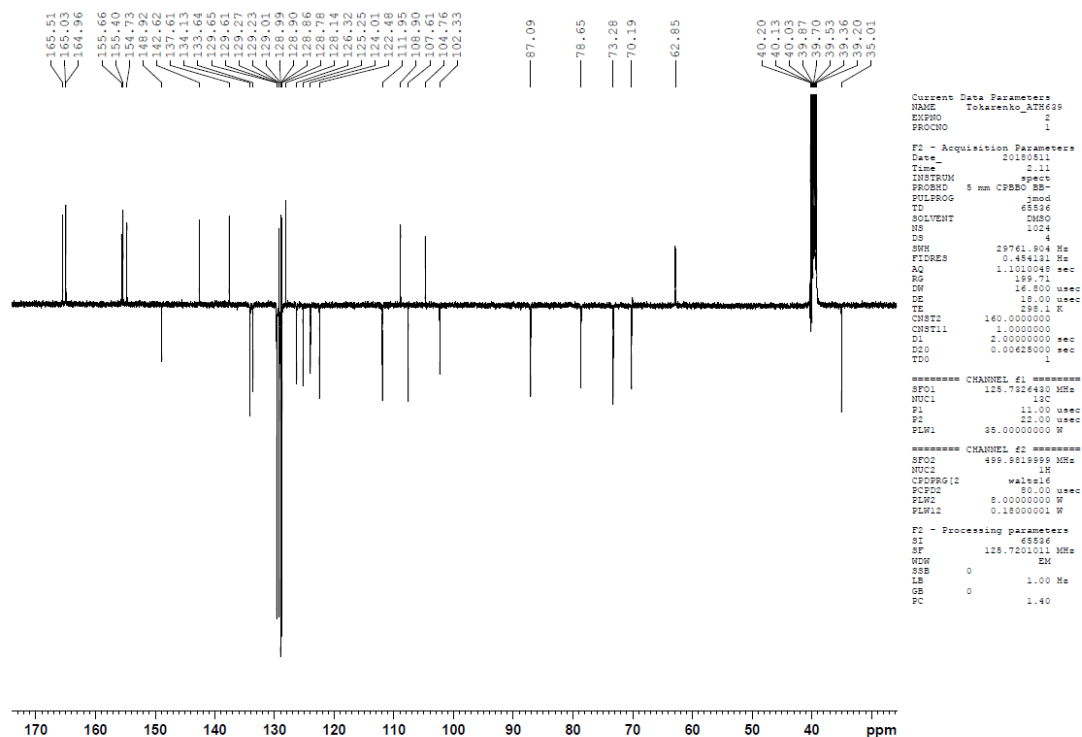
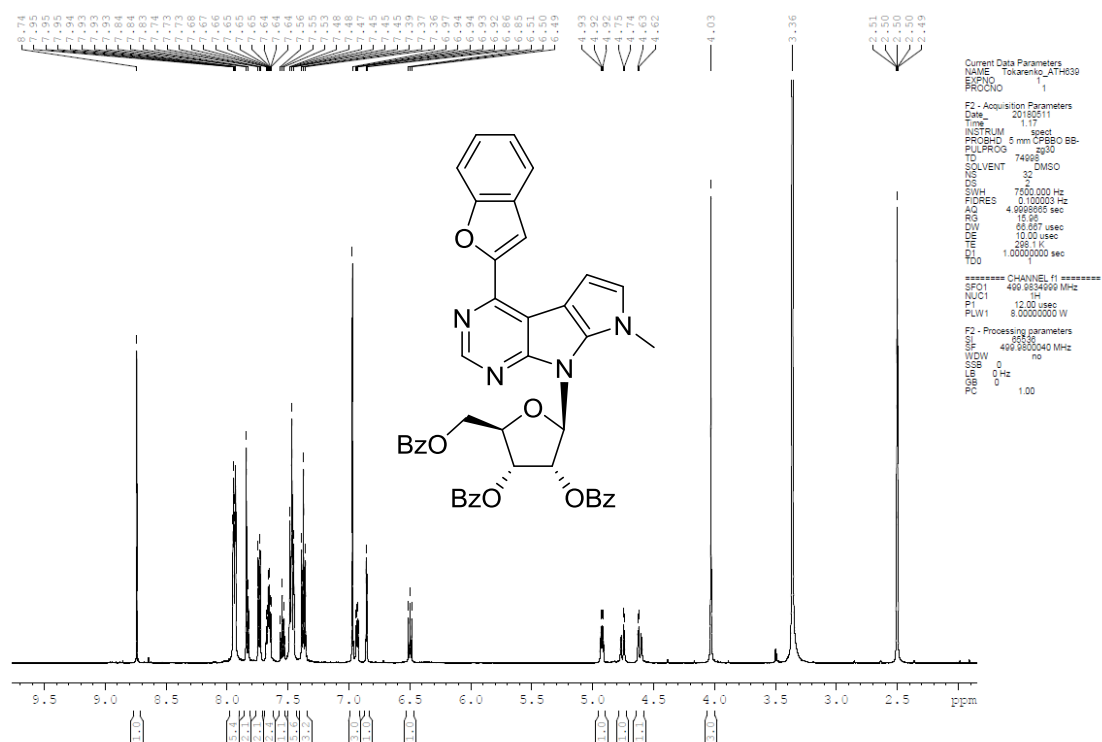
S37



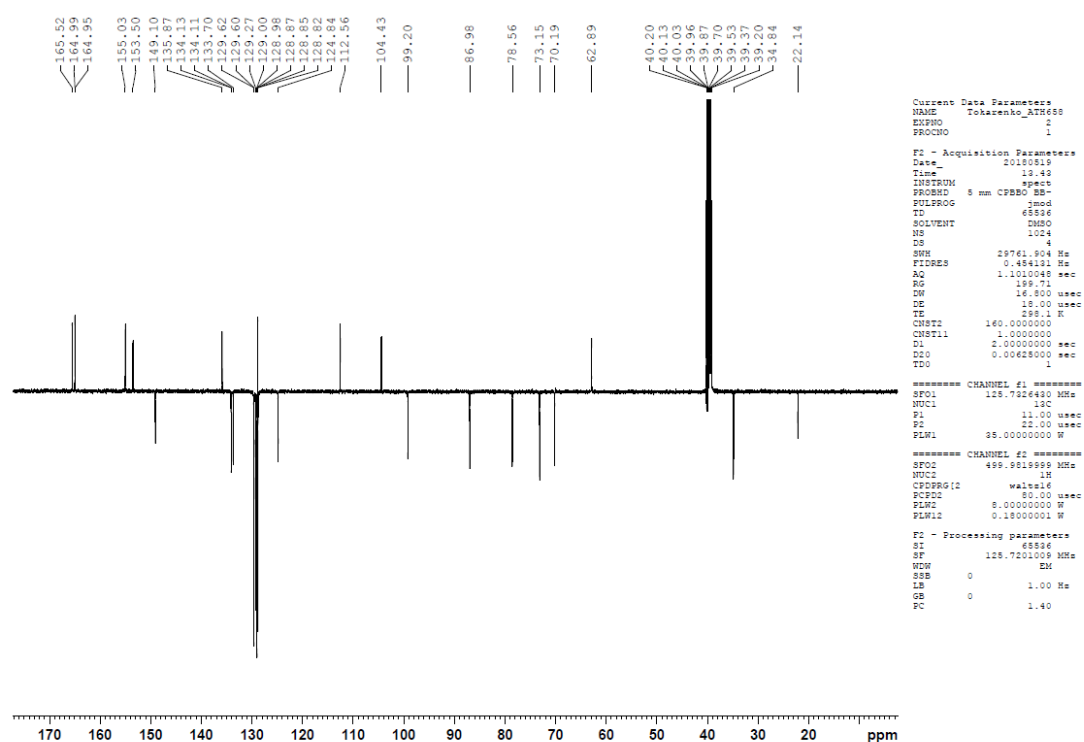
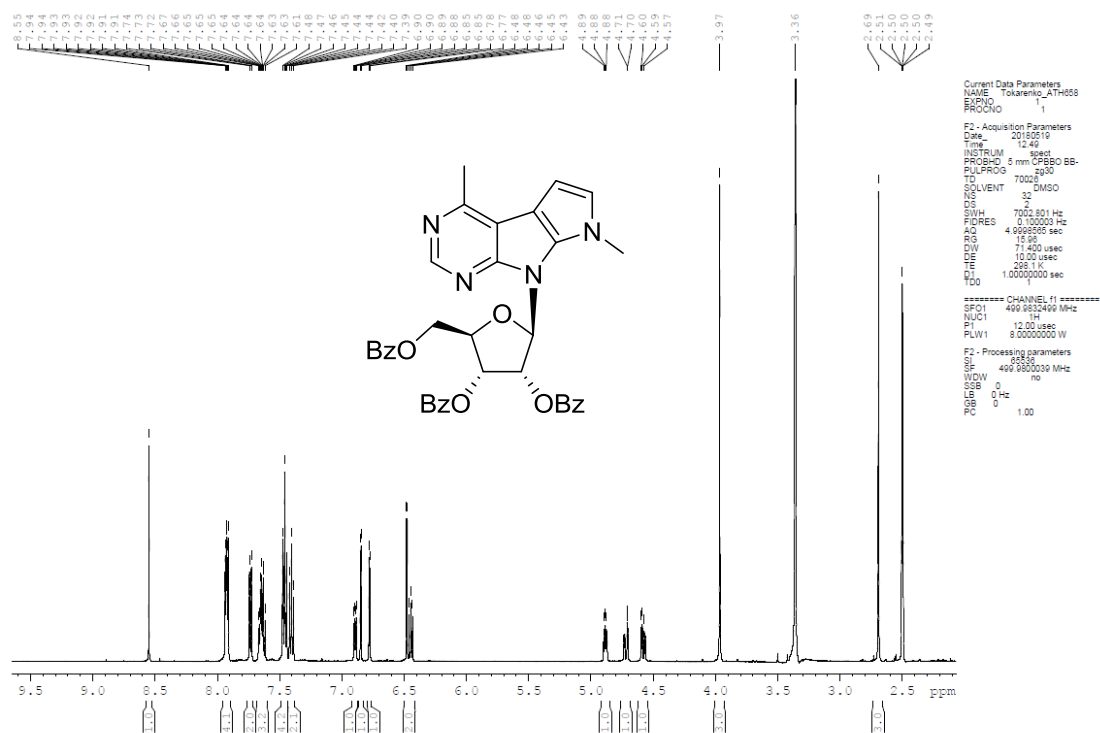
S38



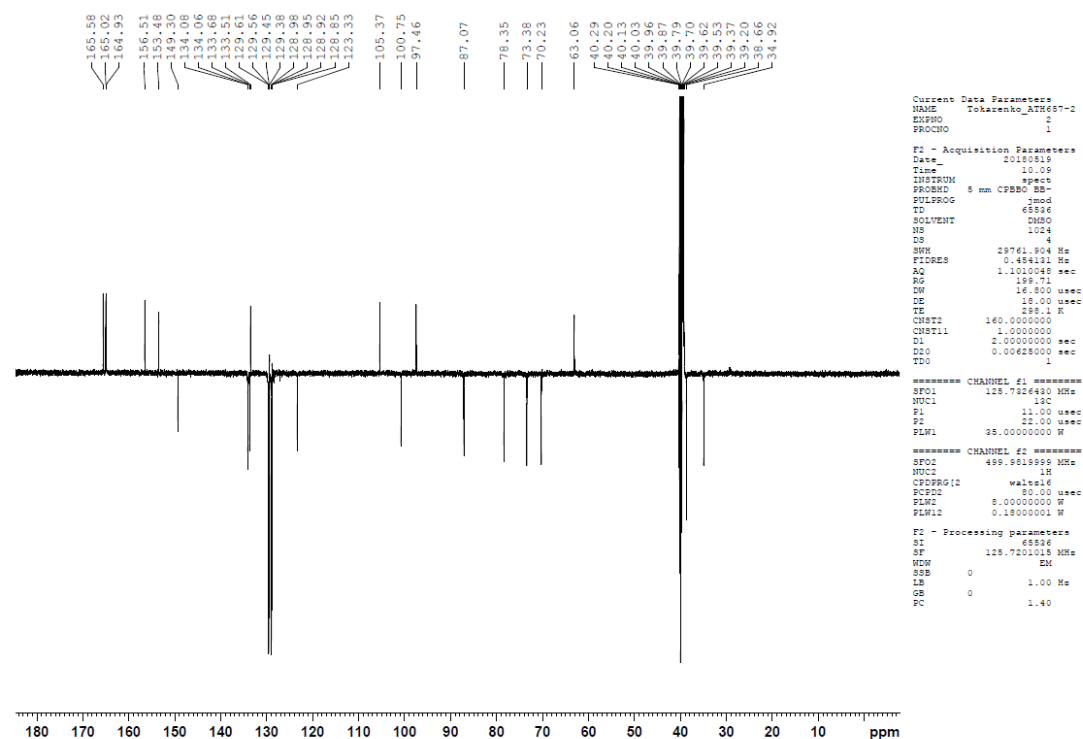
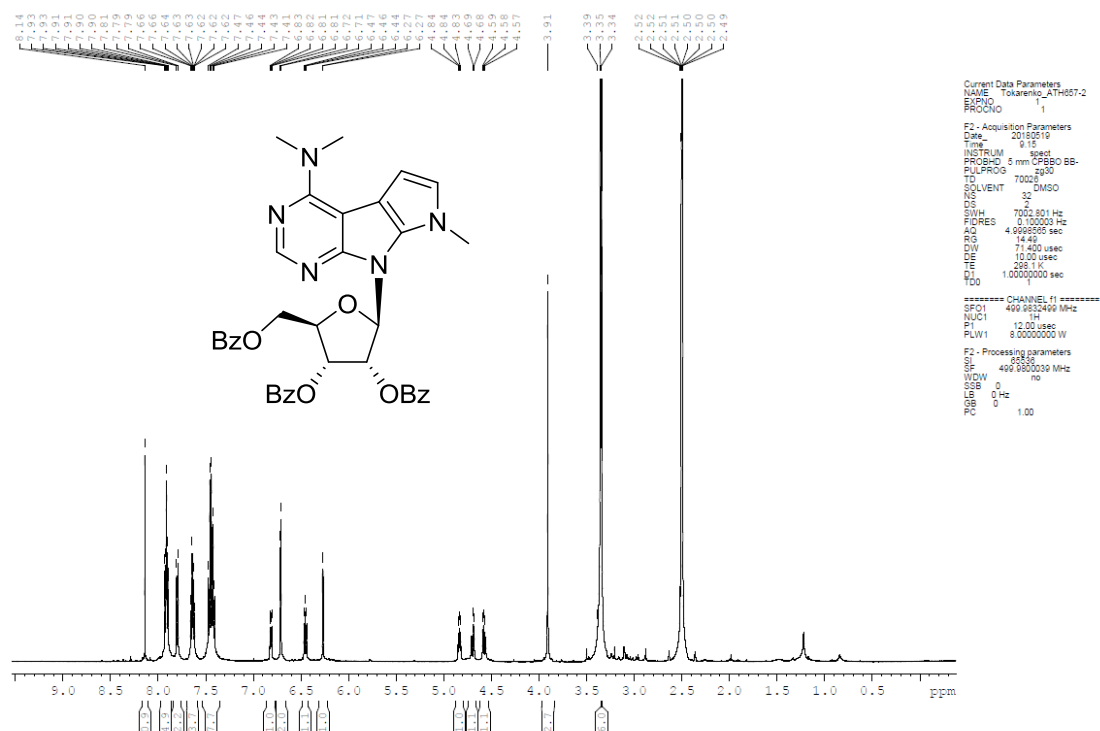
NMR spectra of compound **23c**



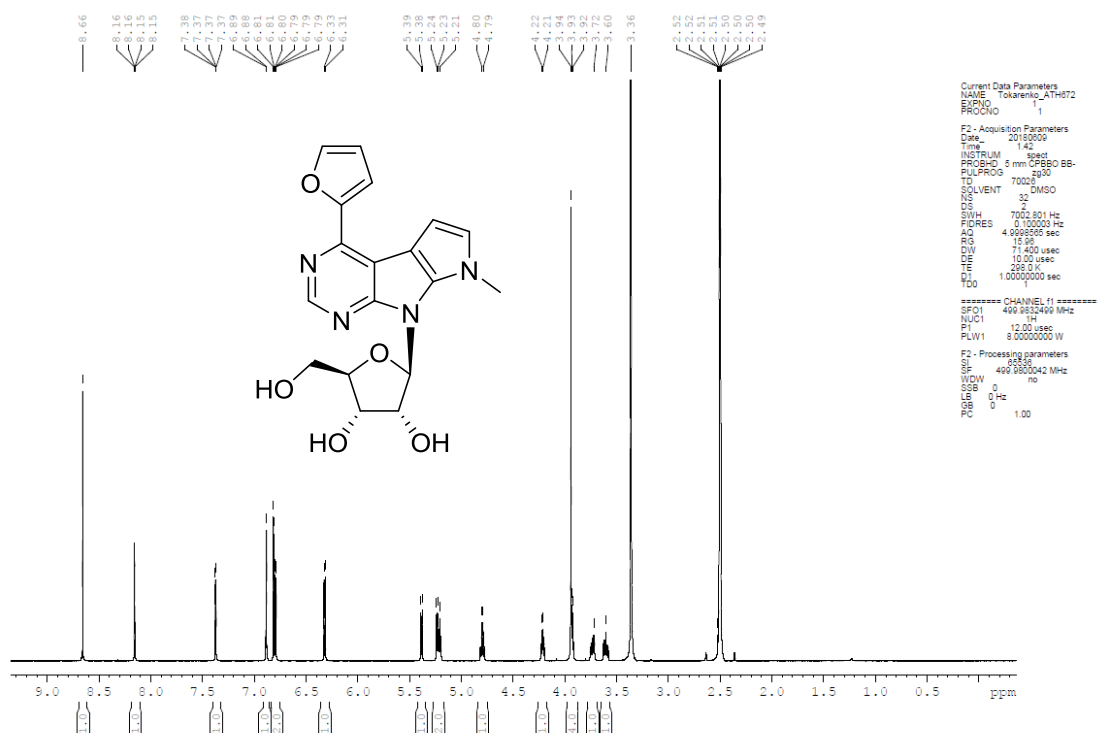
NMR spectra of compound **23d**



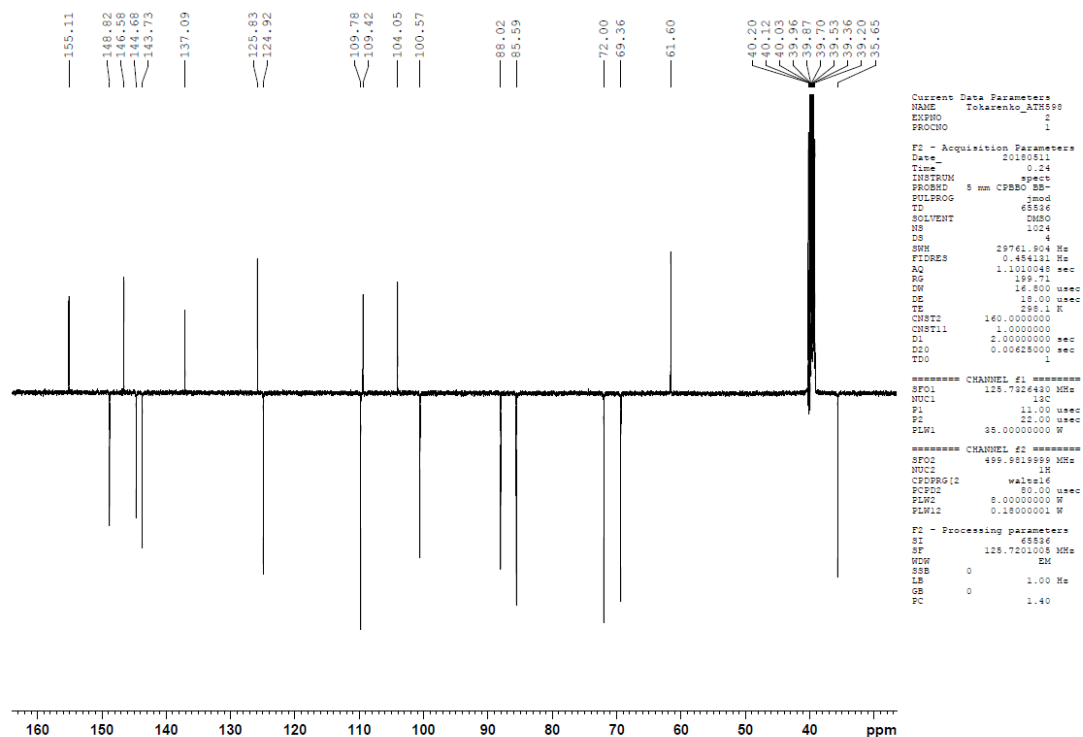
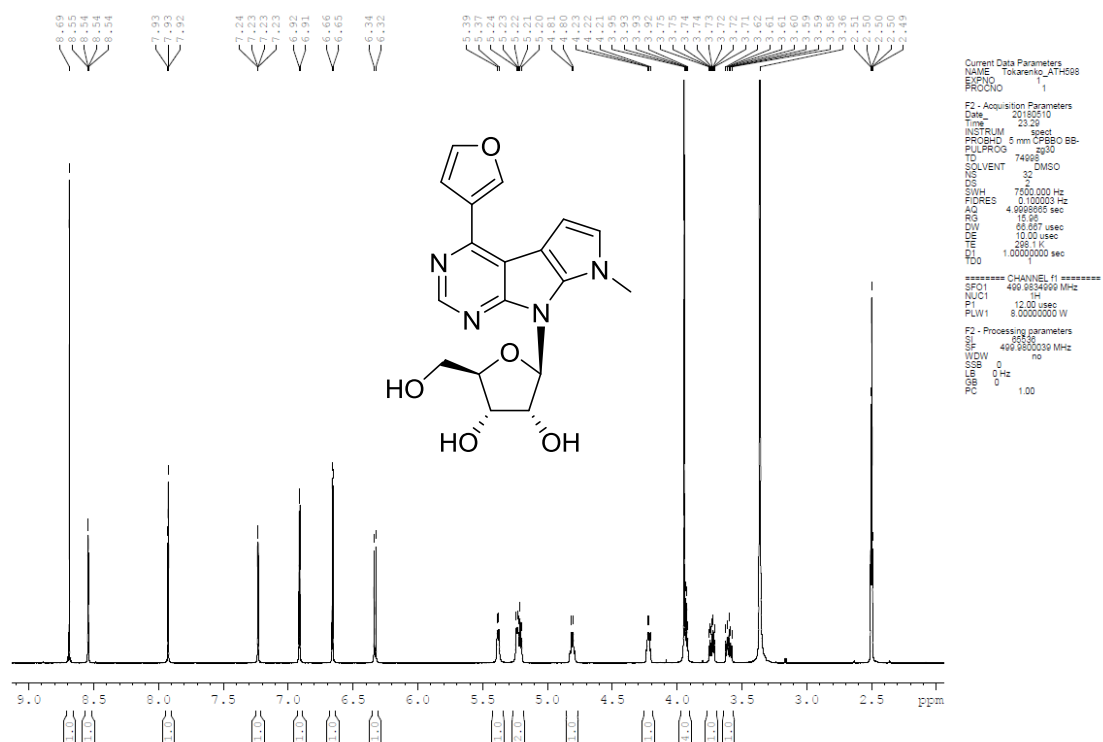
NMR spectra of compound **23e**



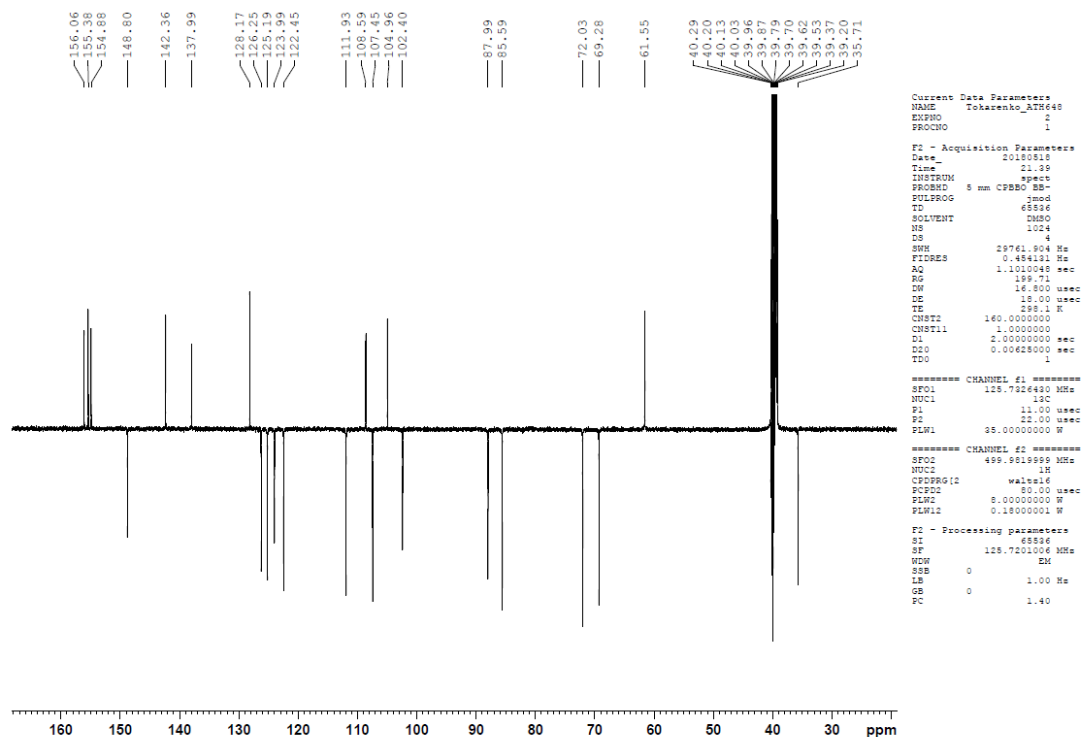
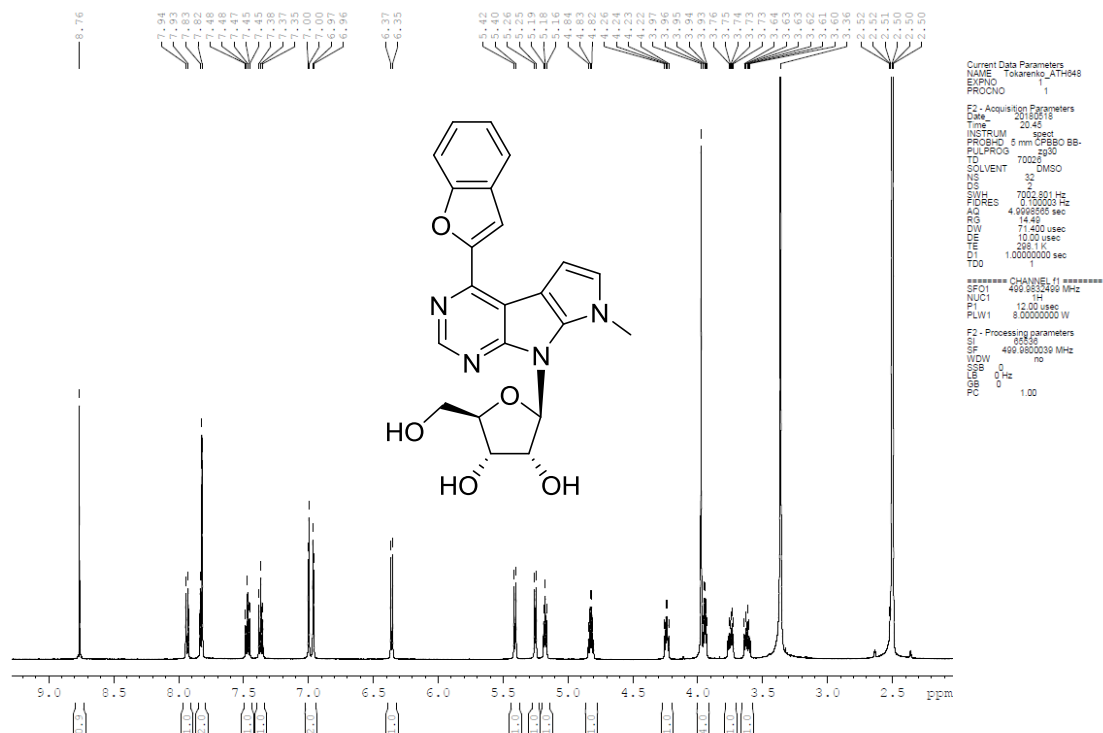
NMR spectra of compound **24a**



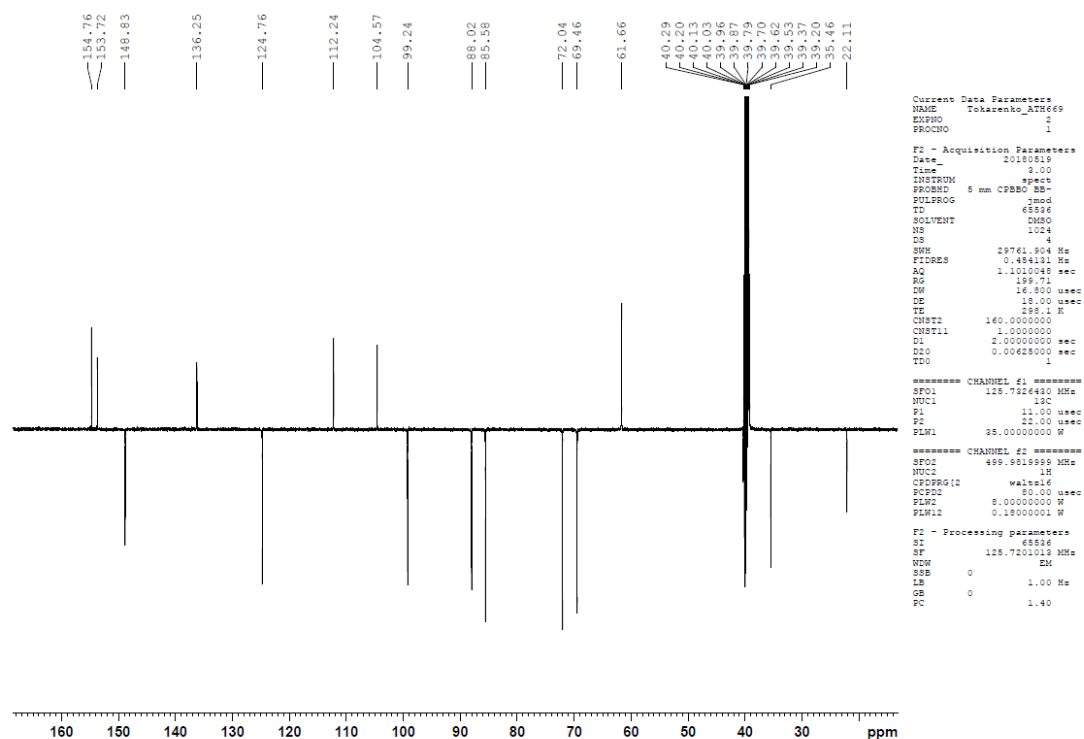
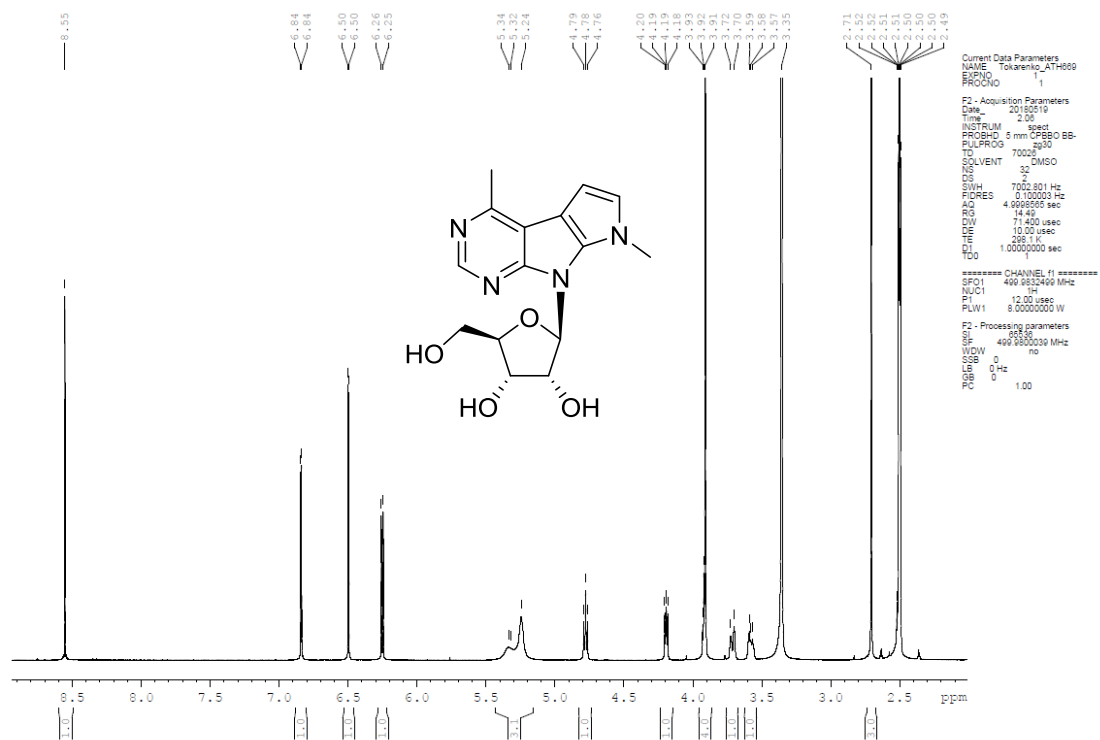
S43



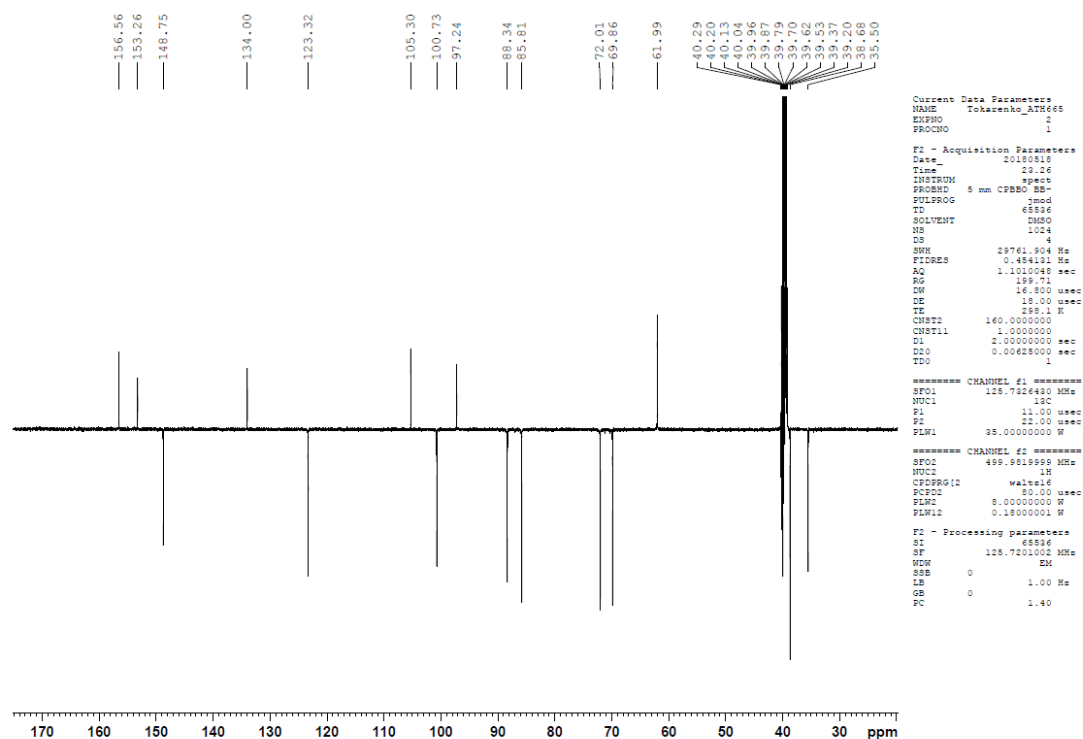
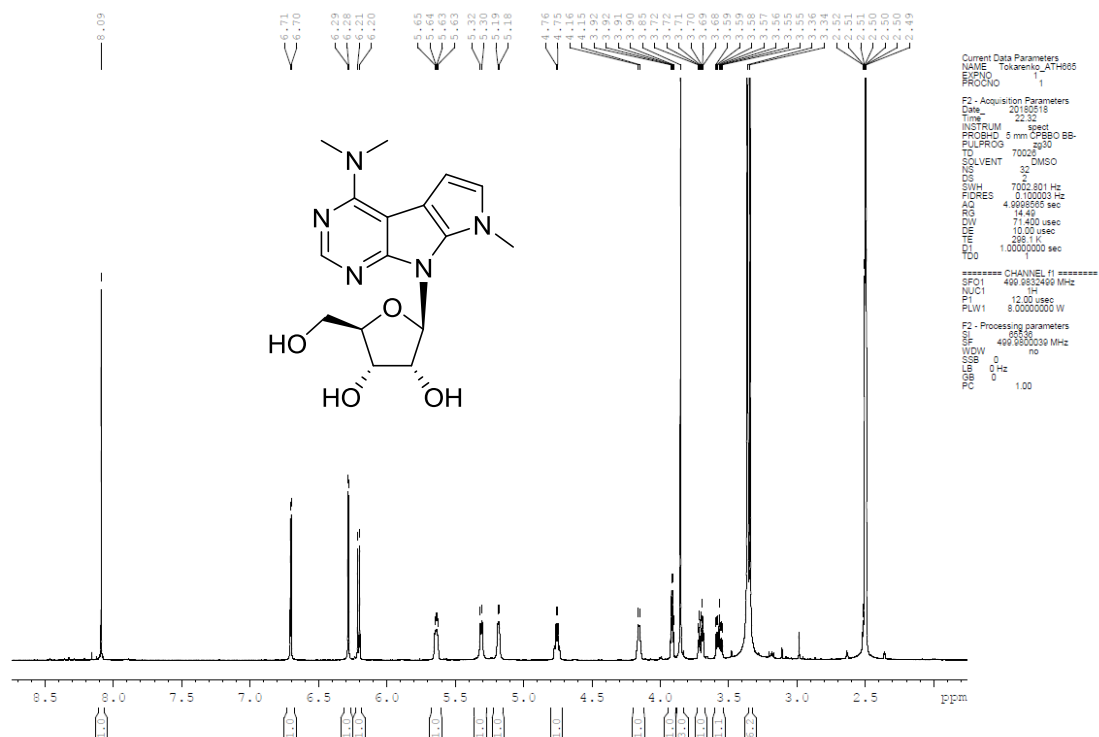
NMR spectra of compound **24c**



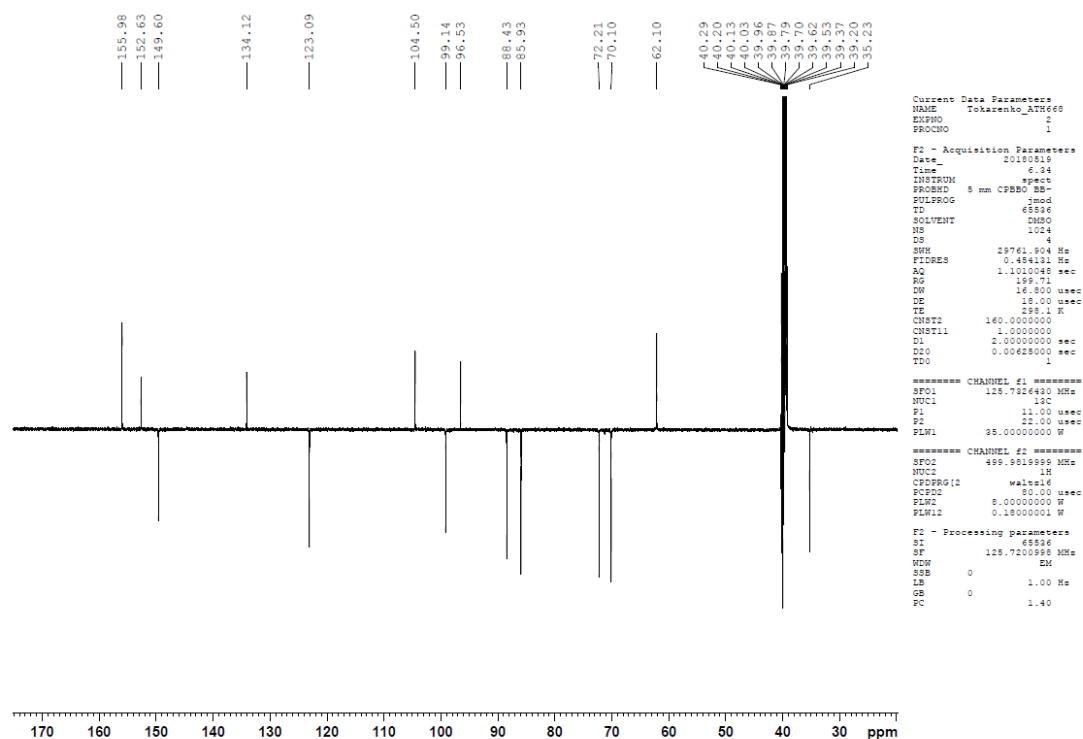
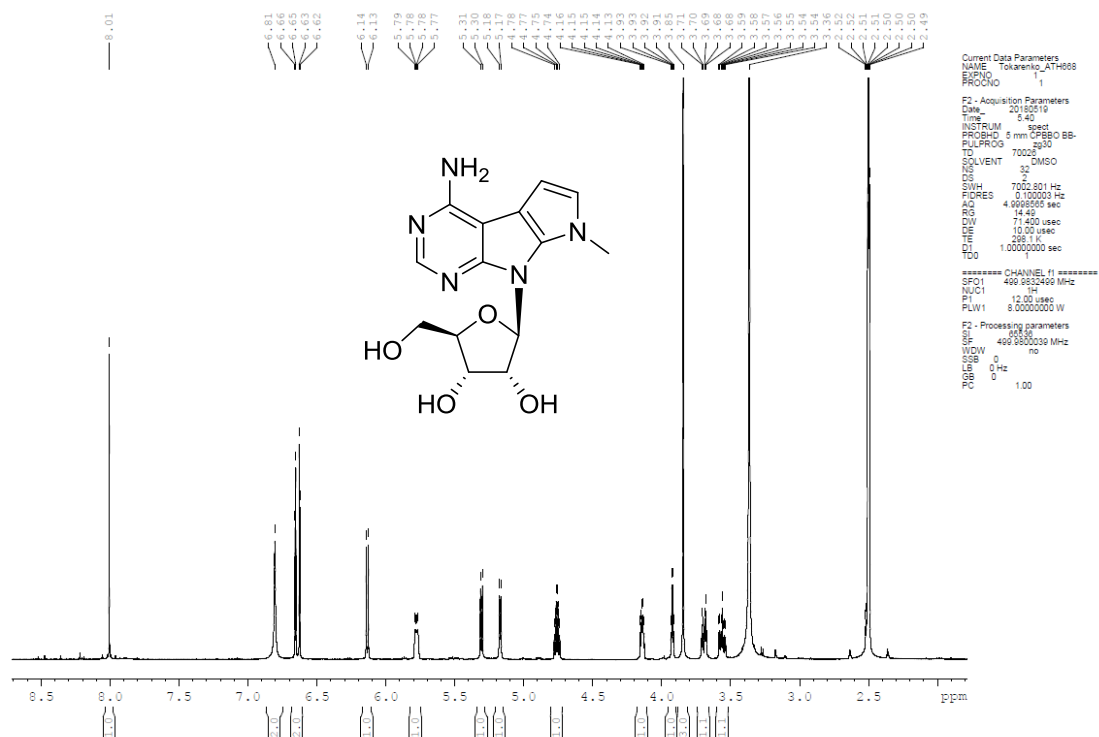
NMR spectra of compound **24d**



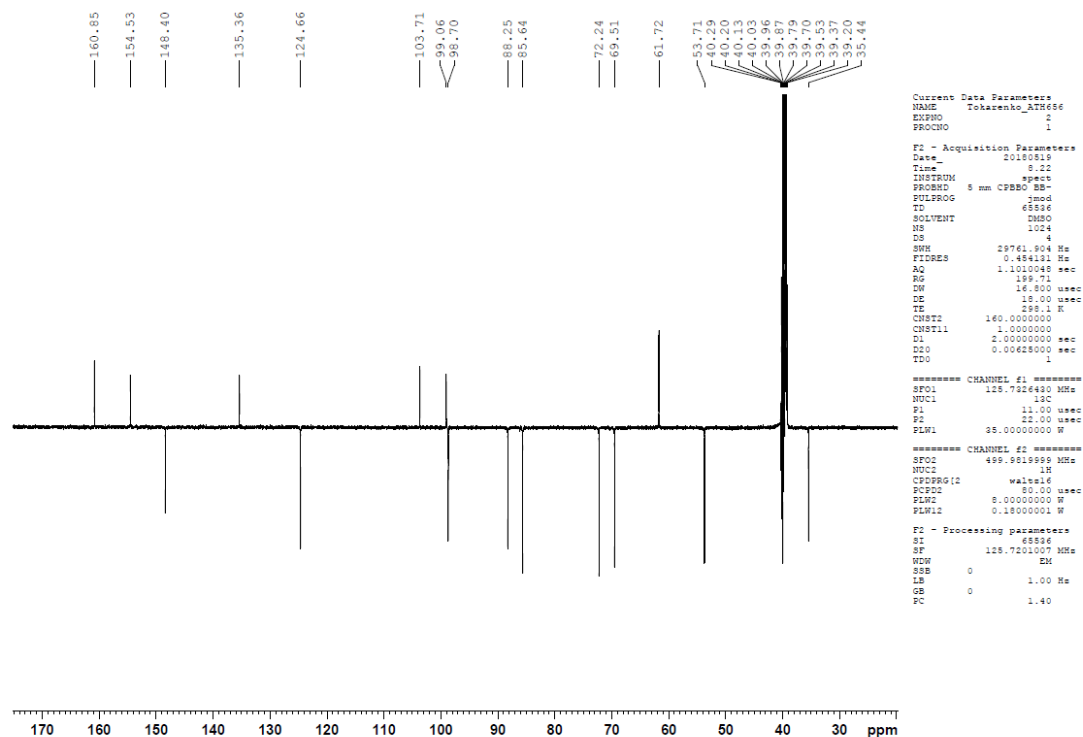
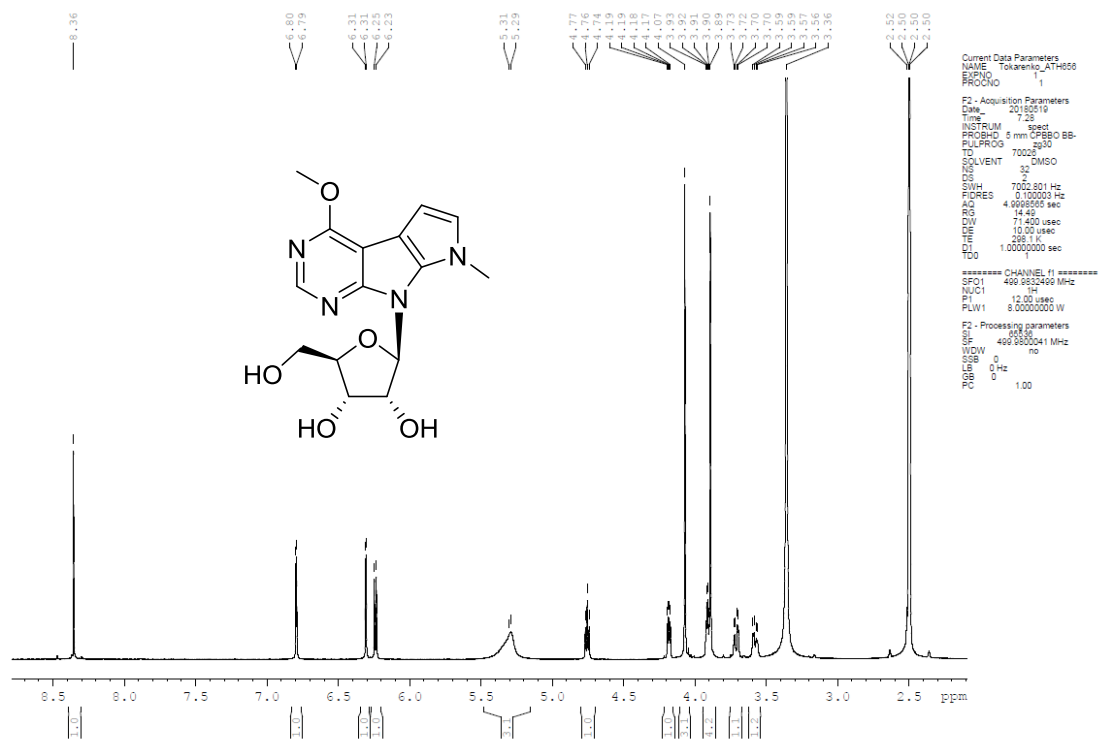
NMR spectra of compound **24e**



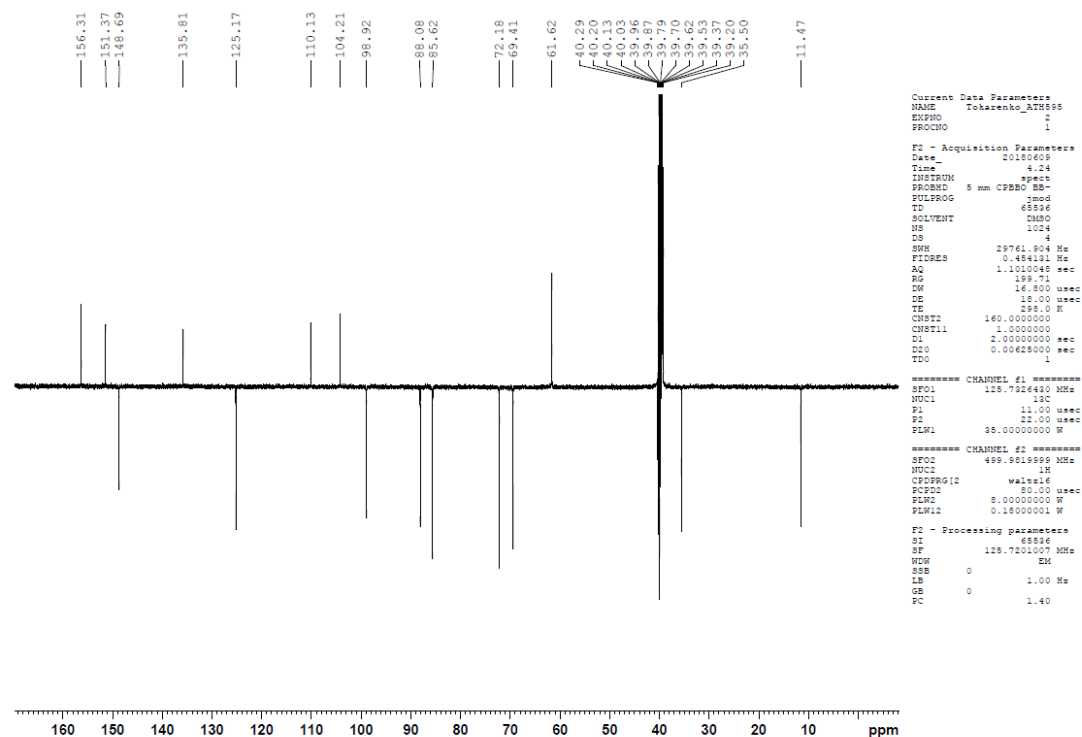
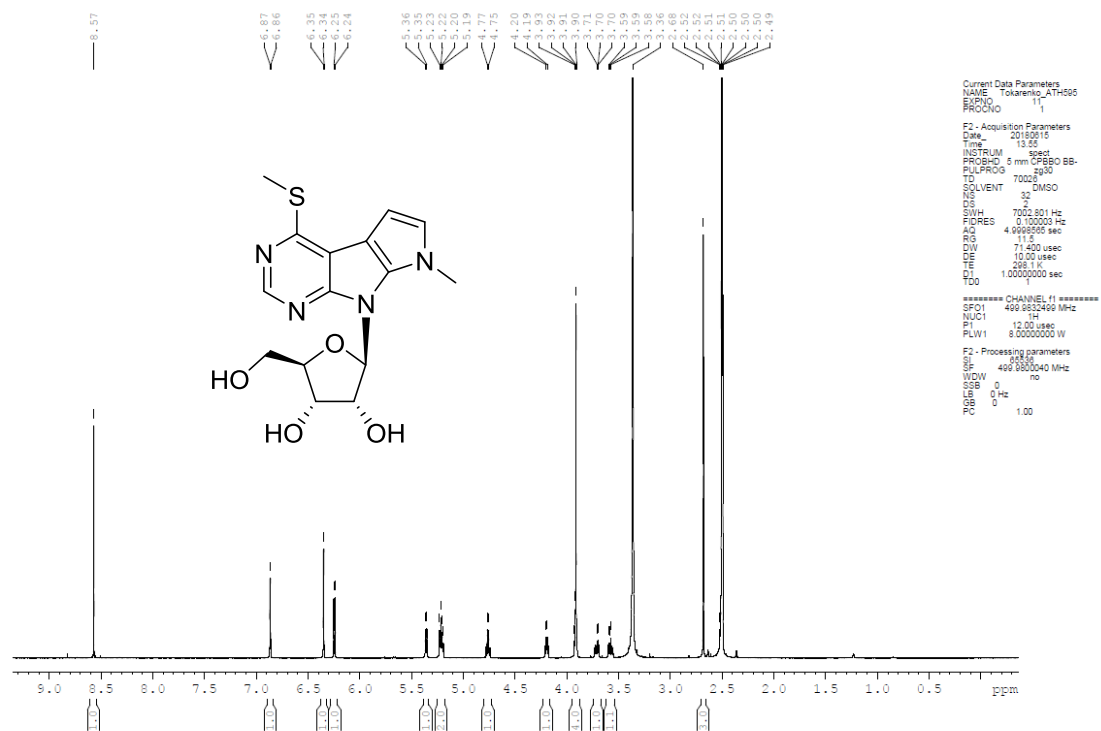
S47



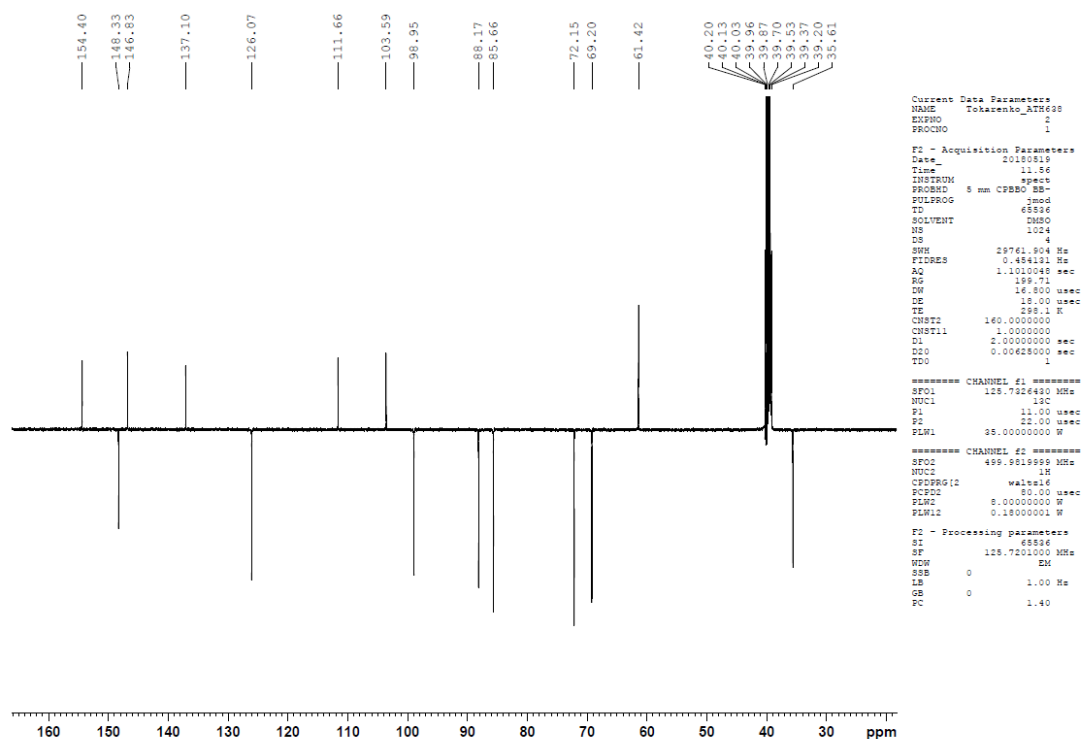
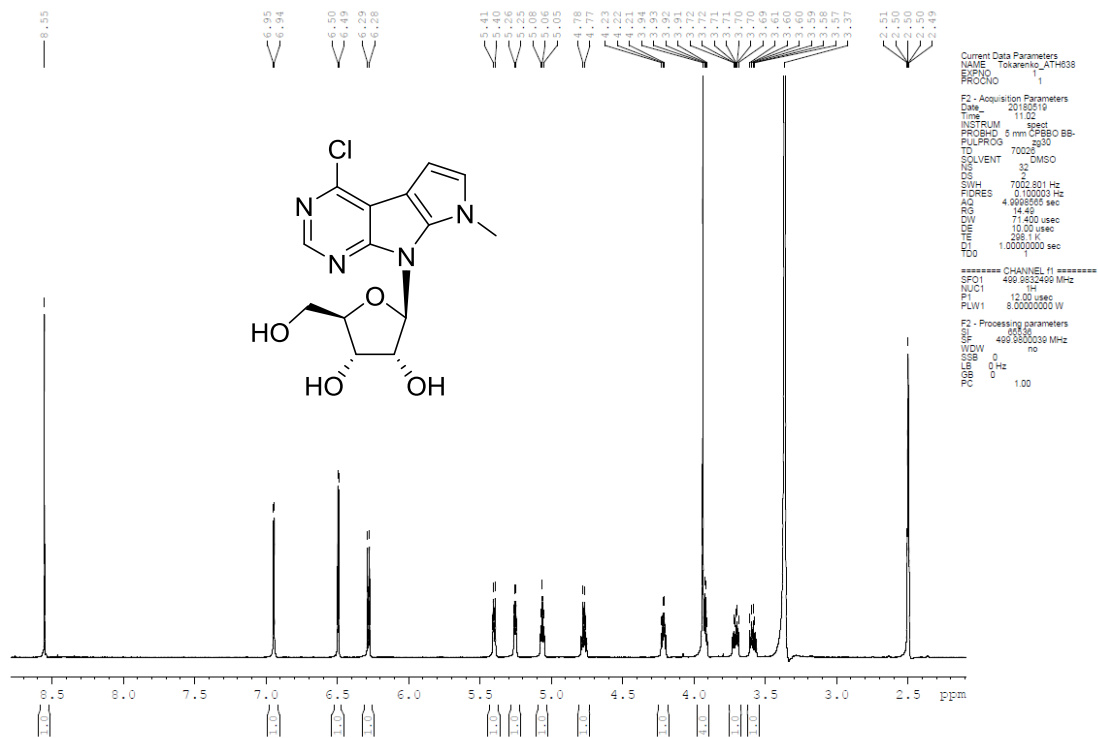
NMR spectra of compound **24g**



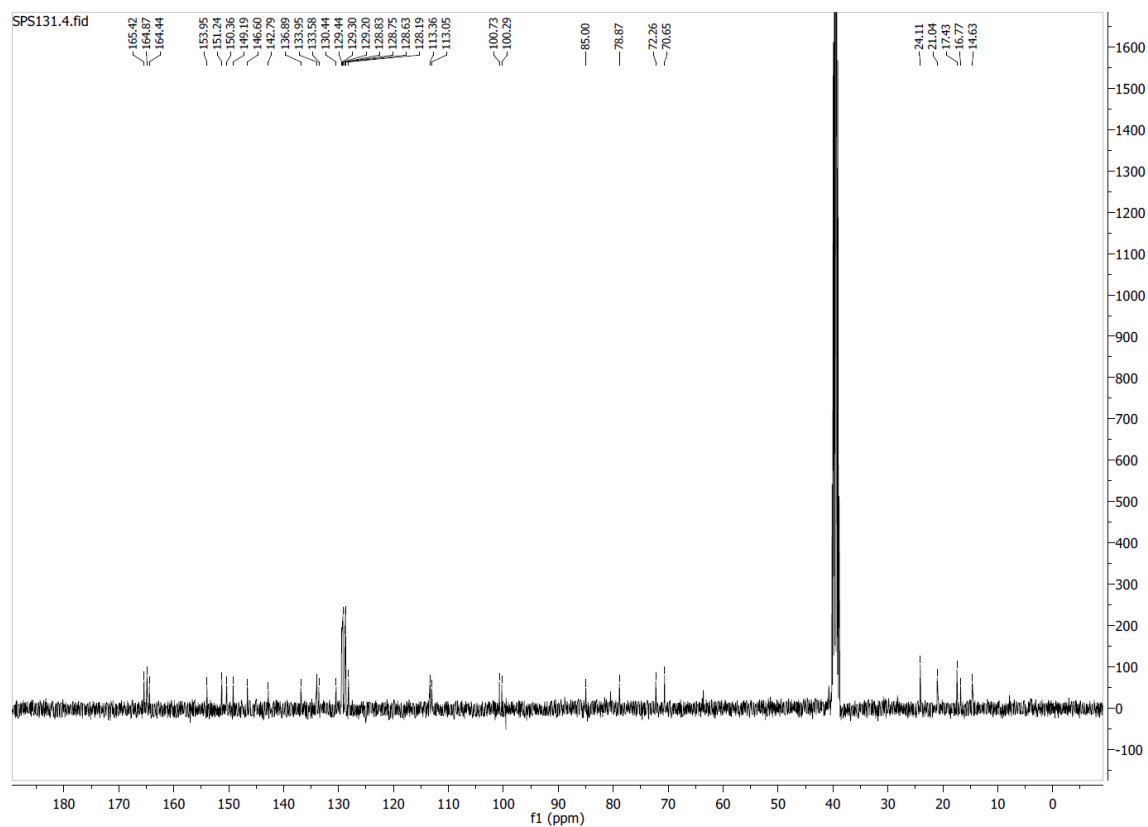
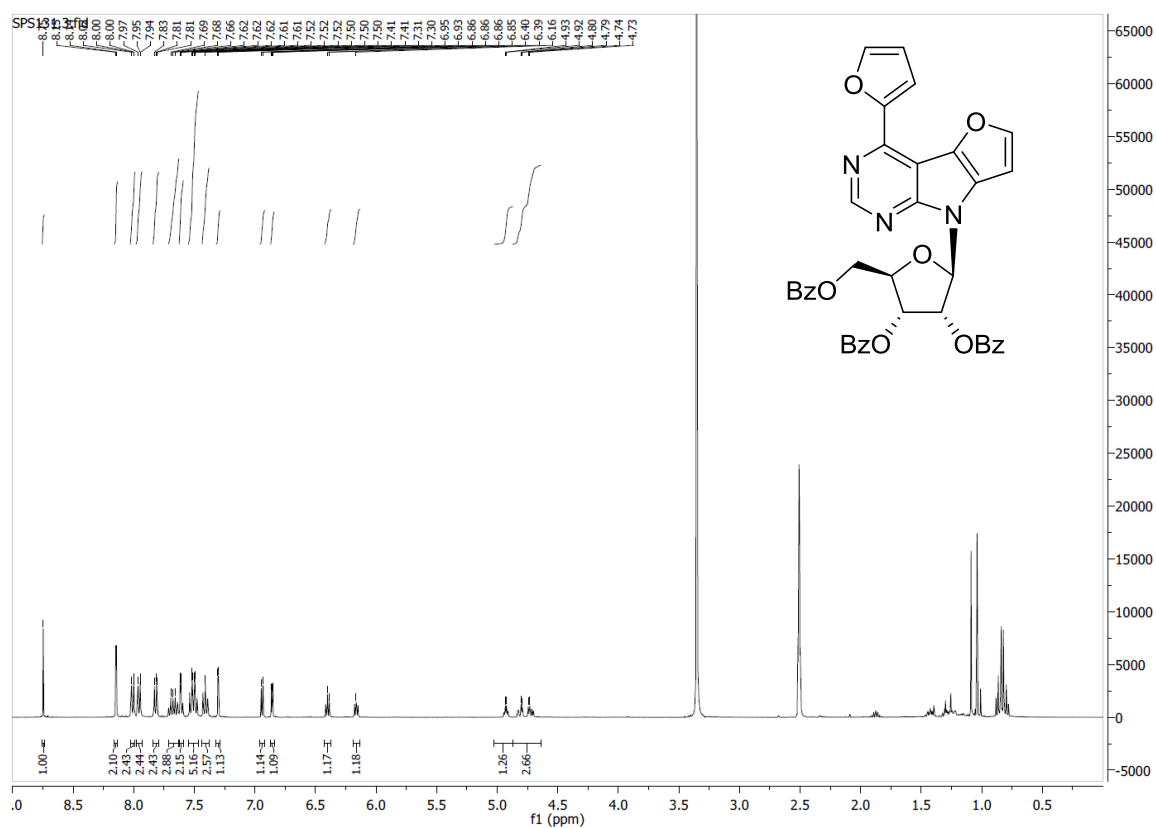
NMR spectra of compound **24h**



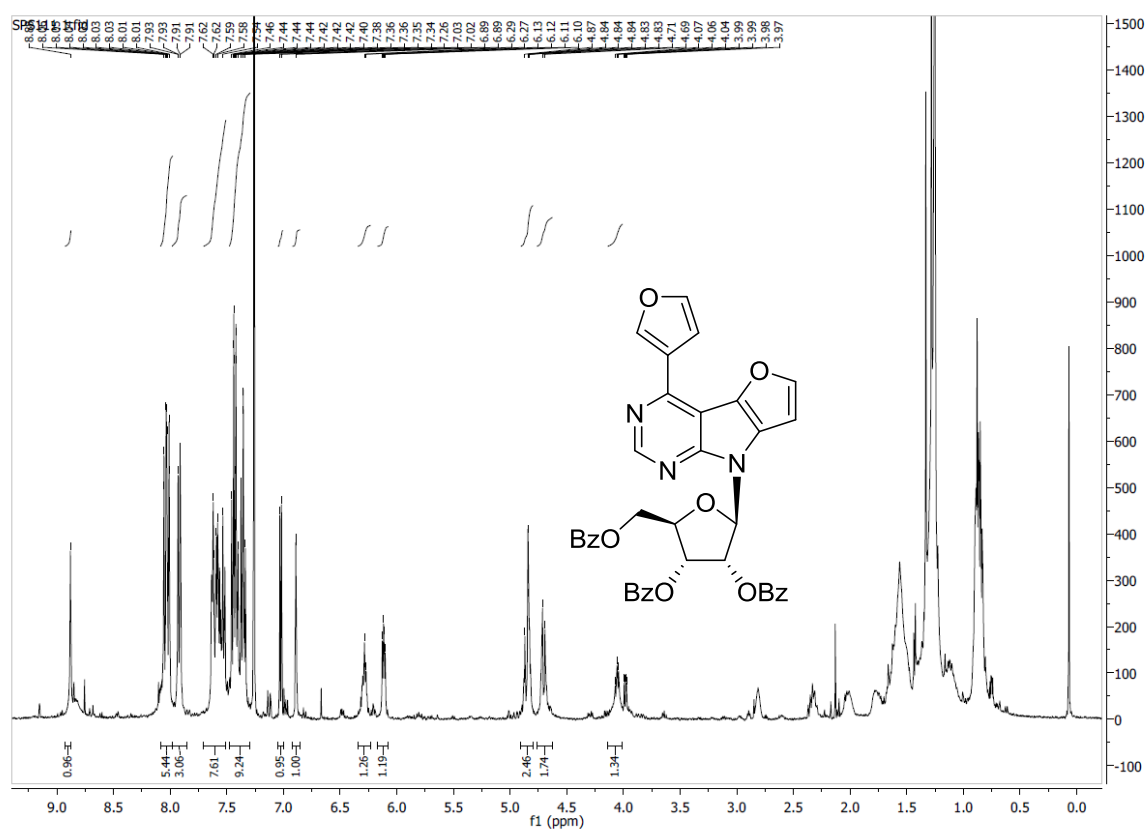
NMR spectra of compound **24i**



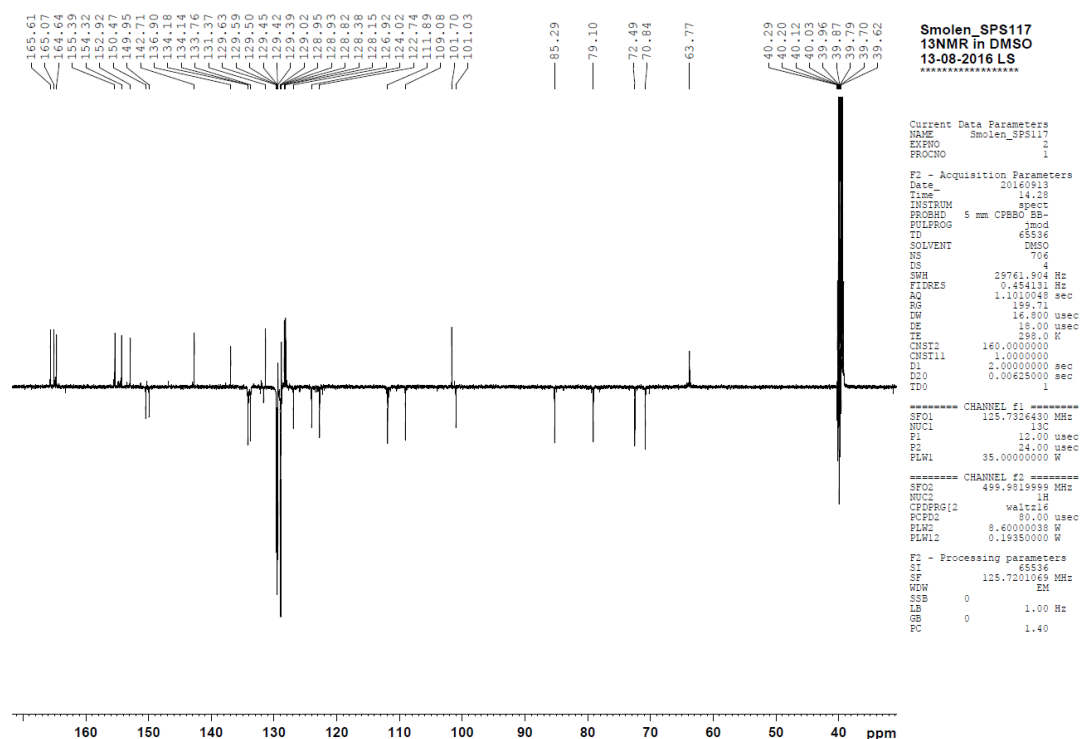
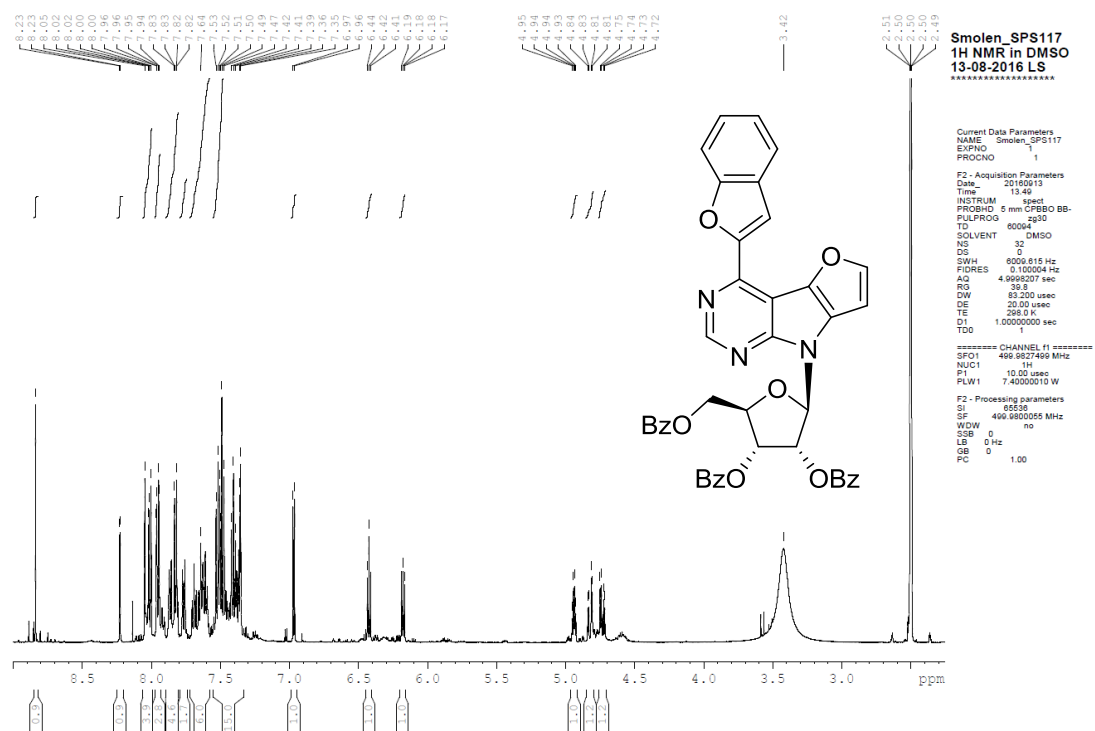
NMR spectra of compound **25a**



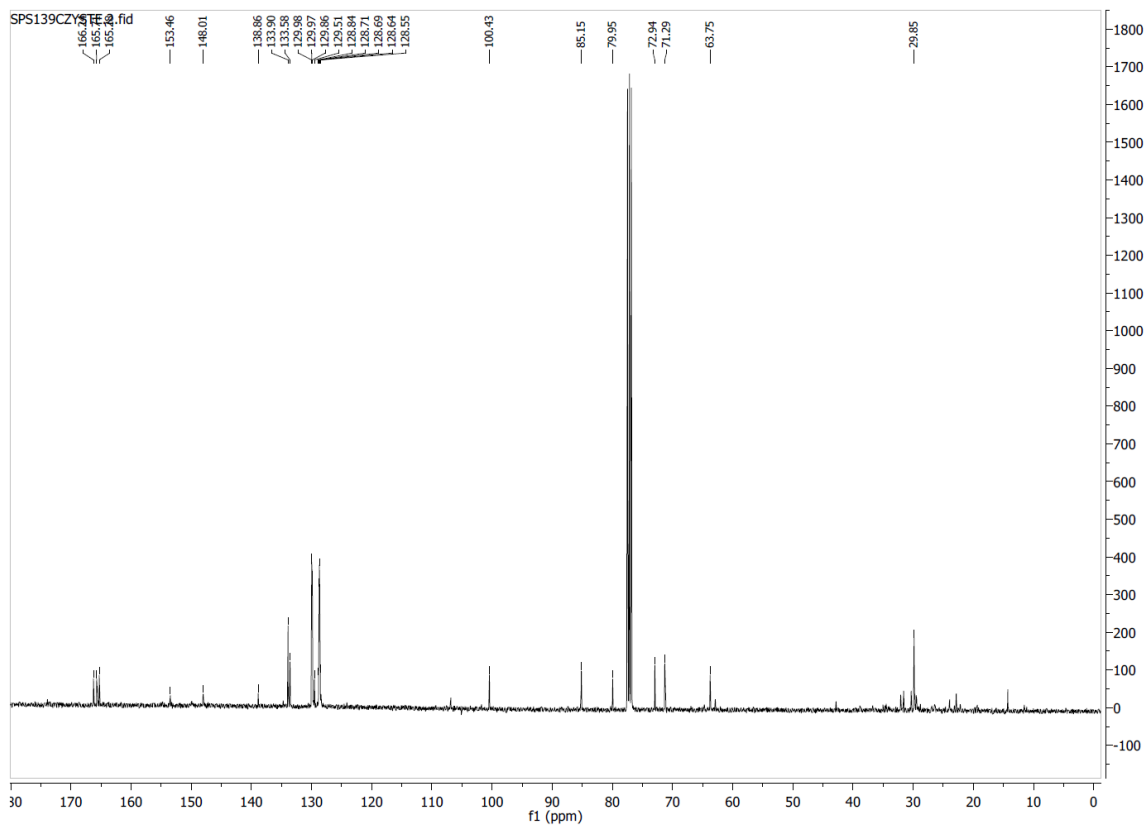
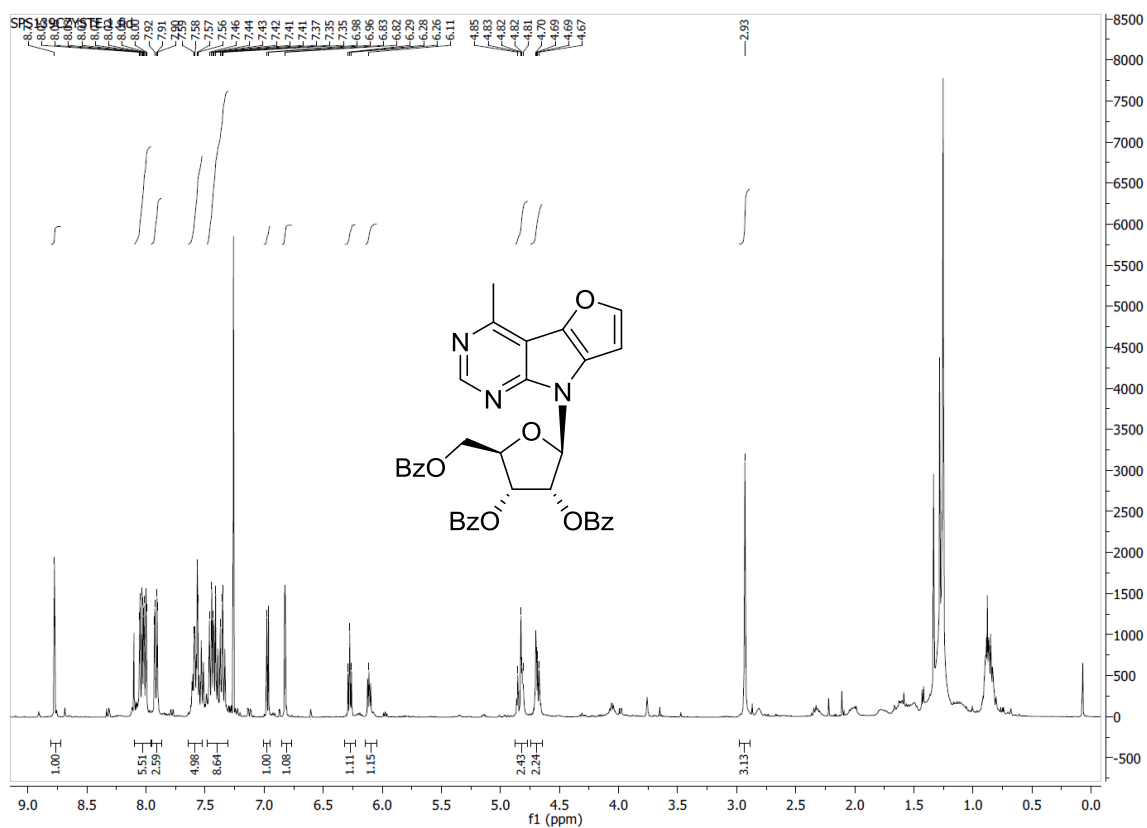
NMR spectrum of compound **25b**



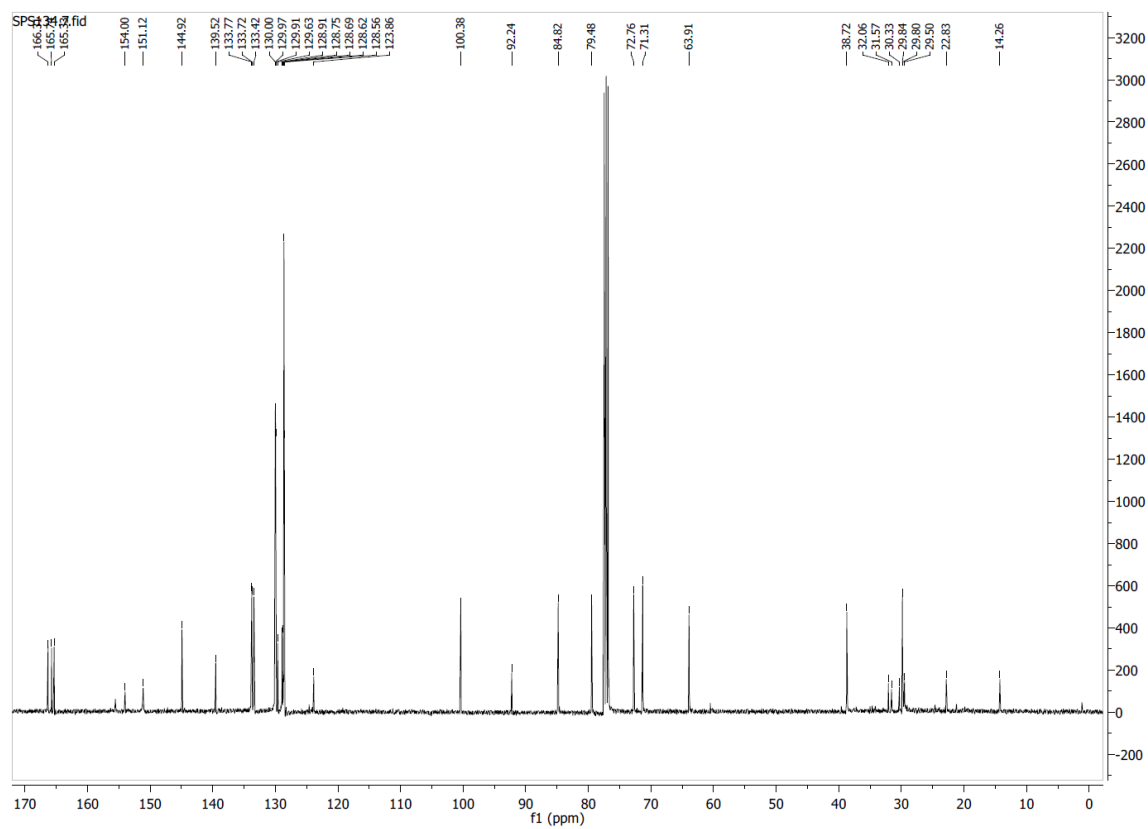
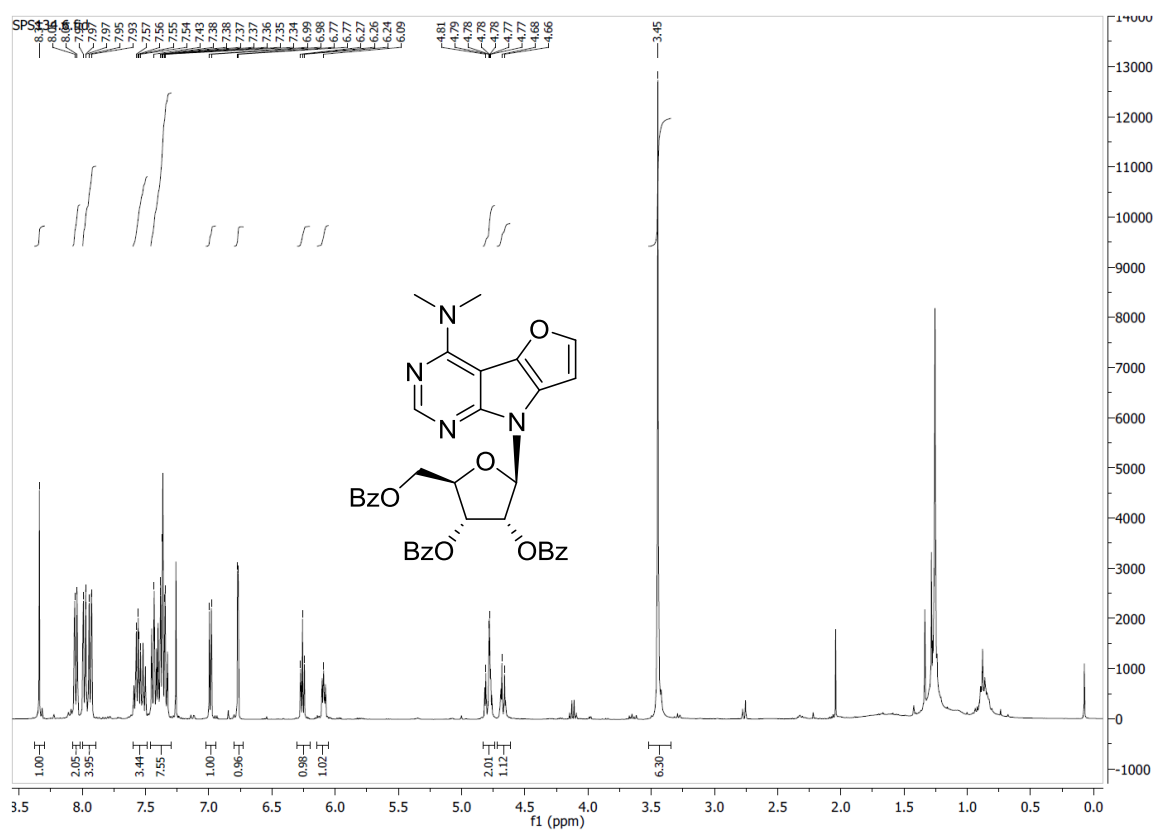
NMR spectra of compound **25c**



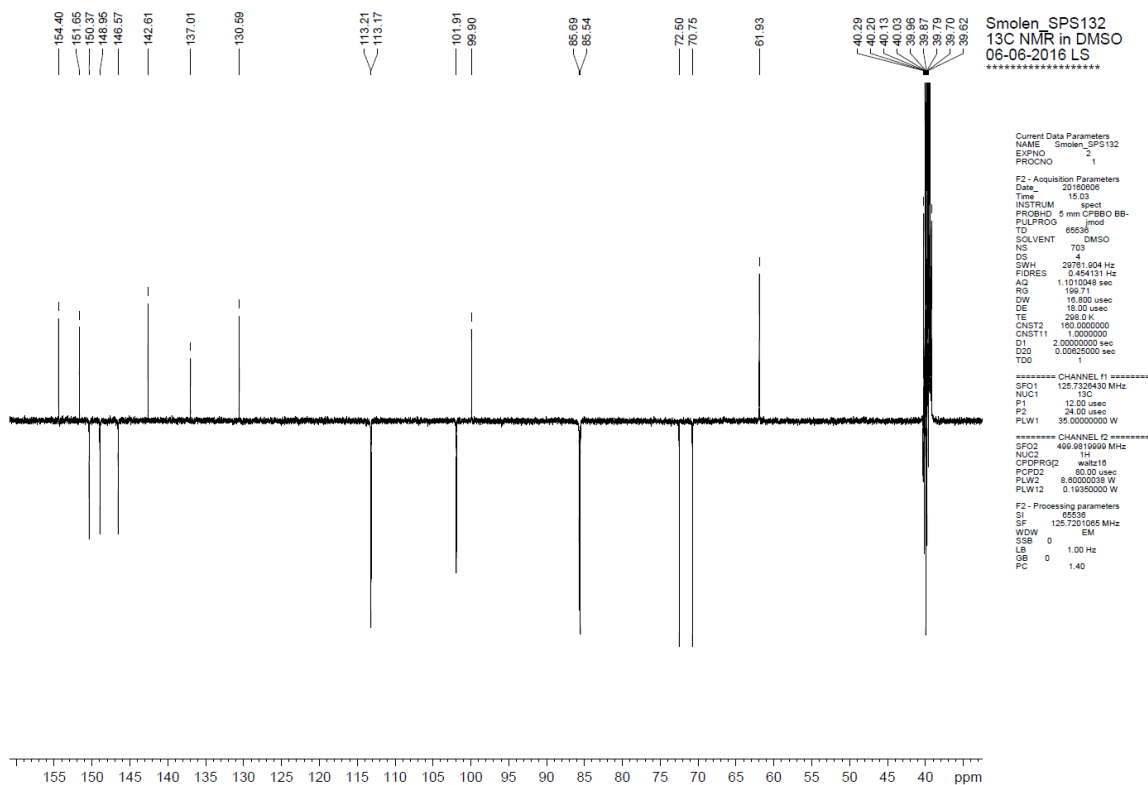
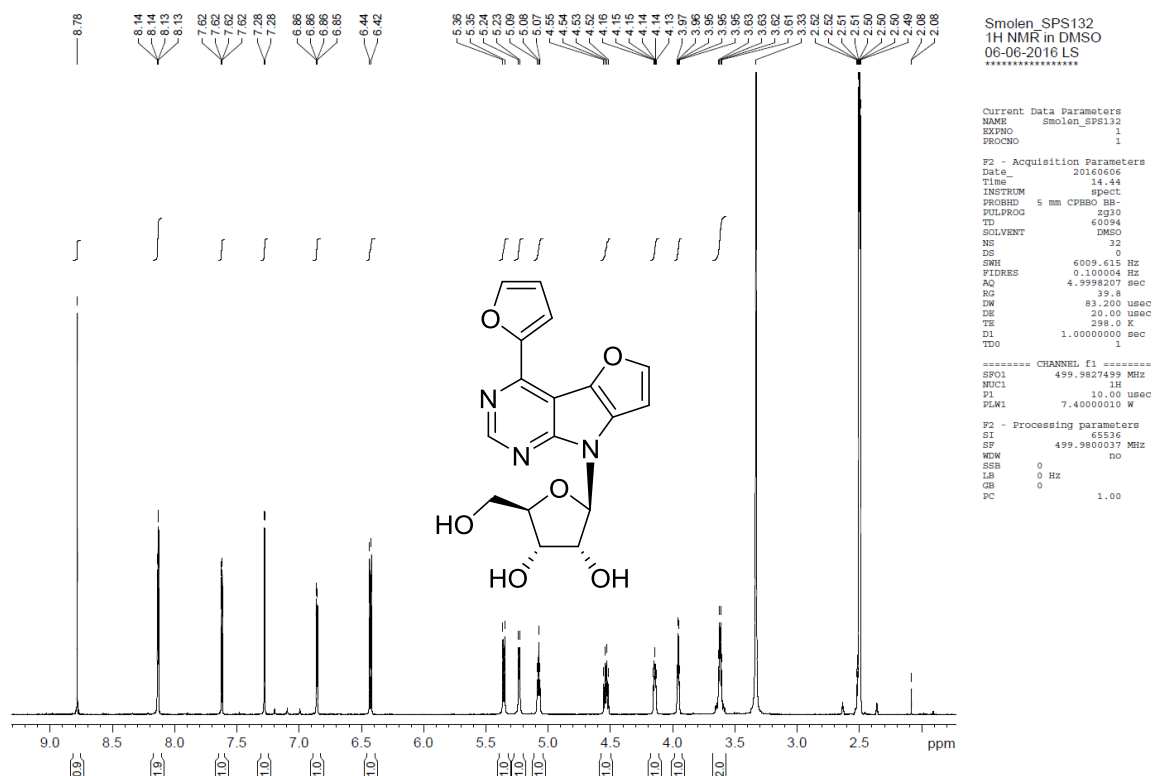
NMR spectra of compound **25d**



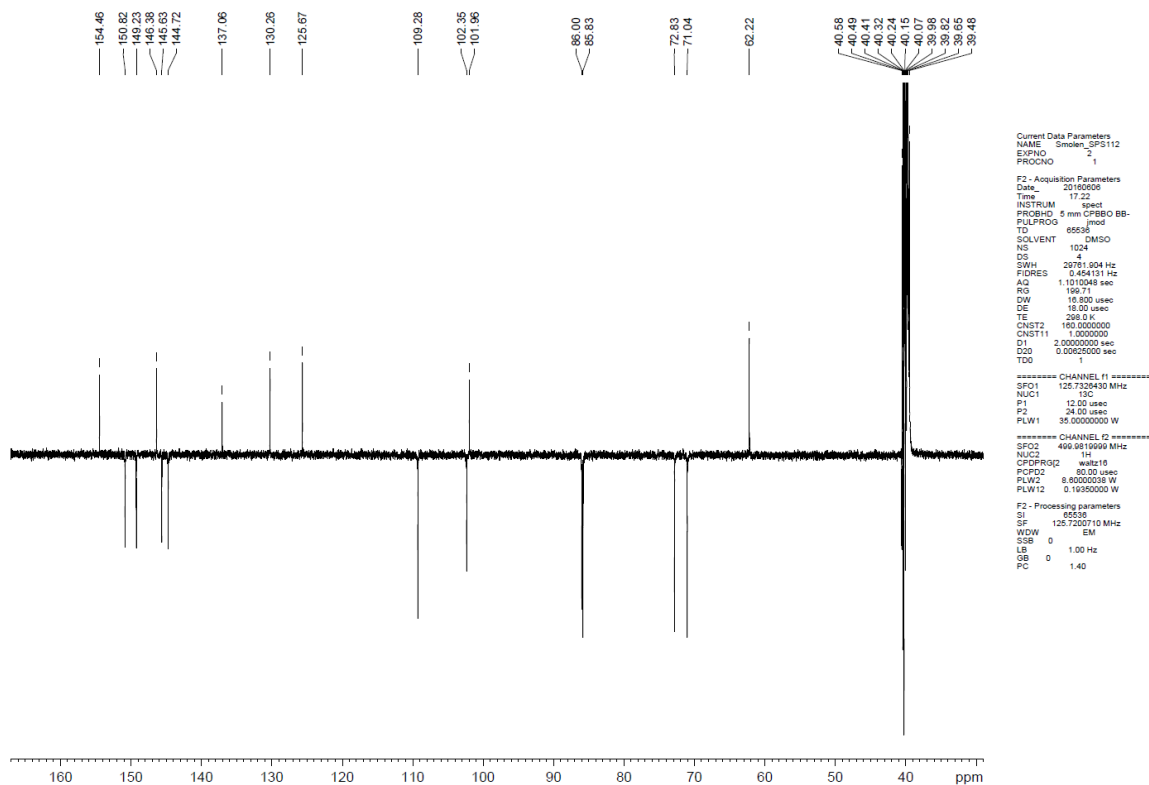
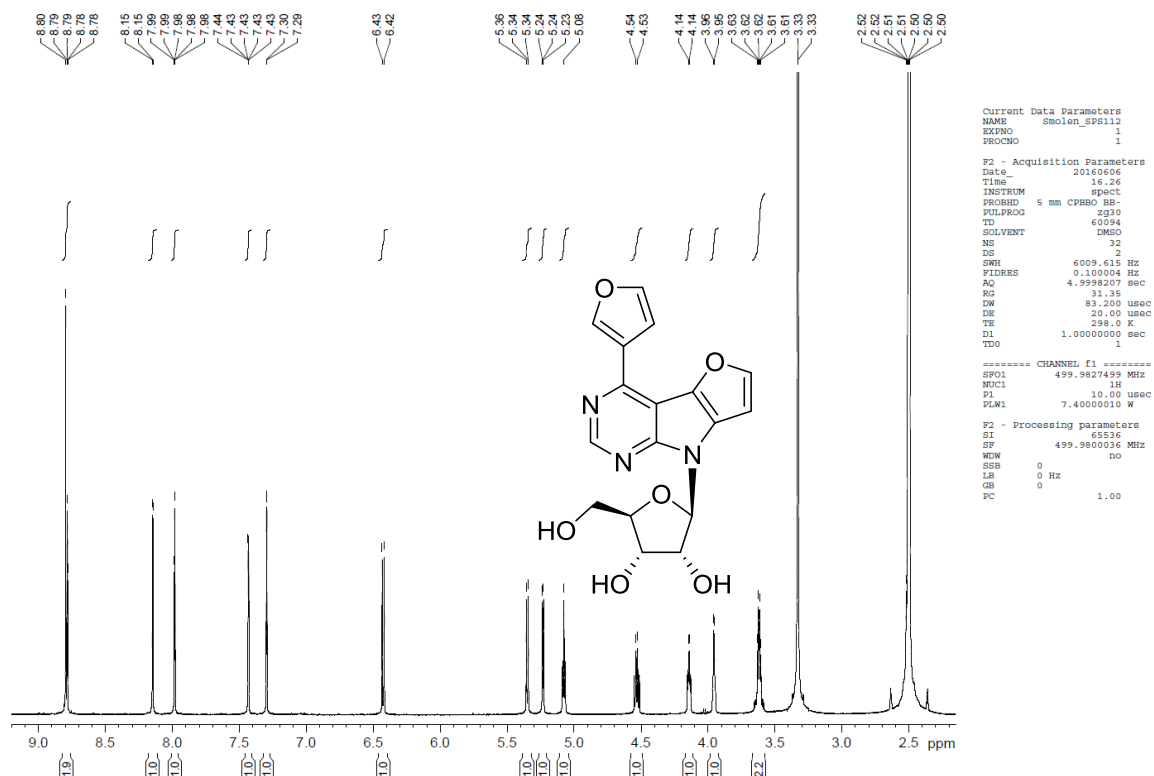
NMR spectra of compound **25e**



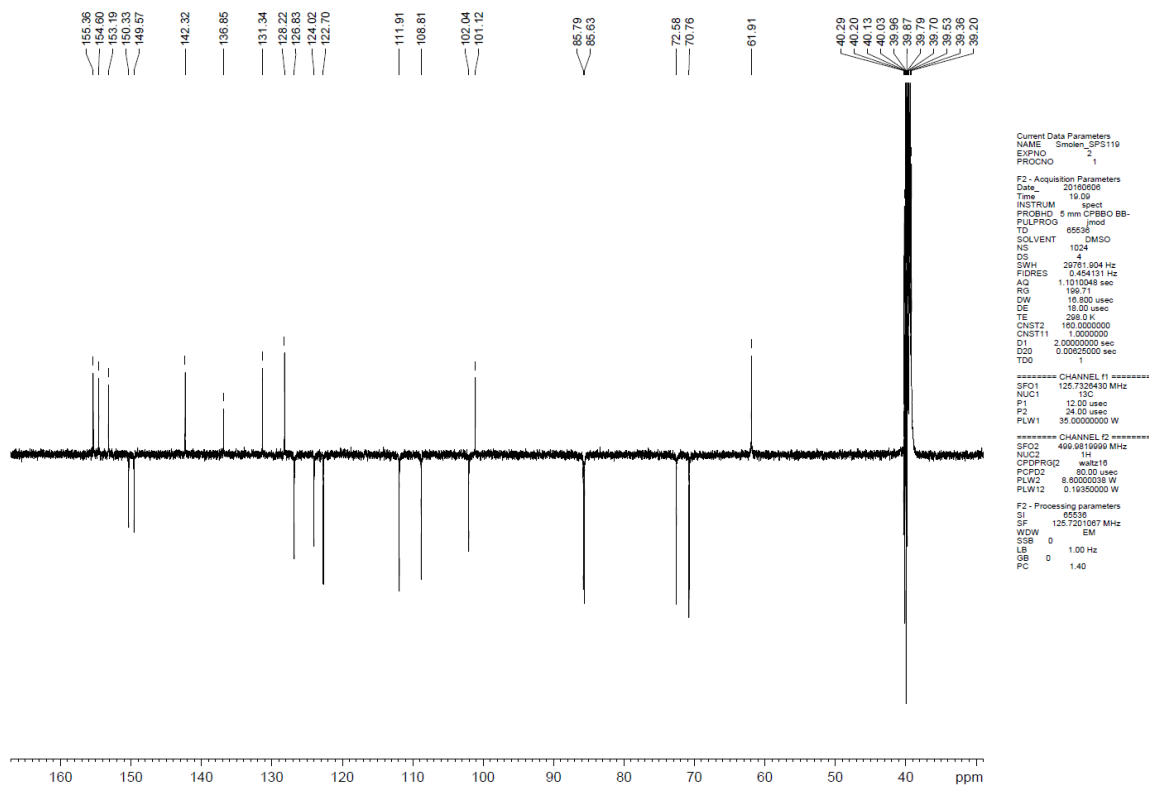
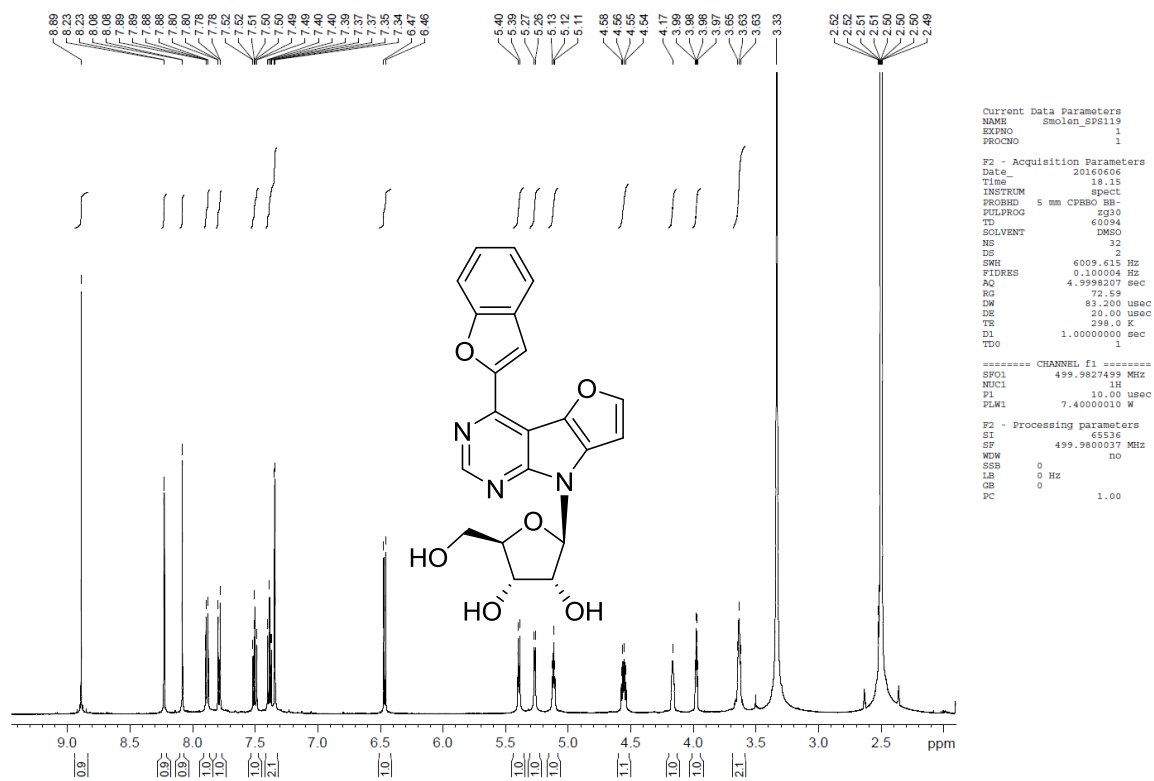
NMR spectra of compound **26a**



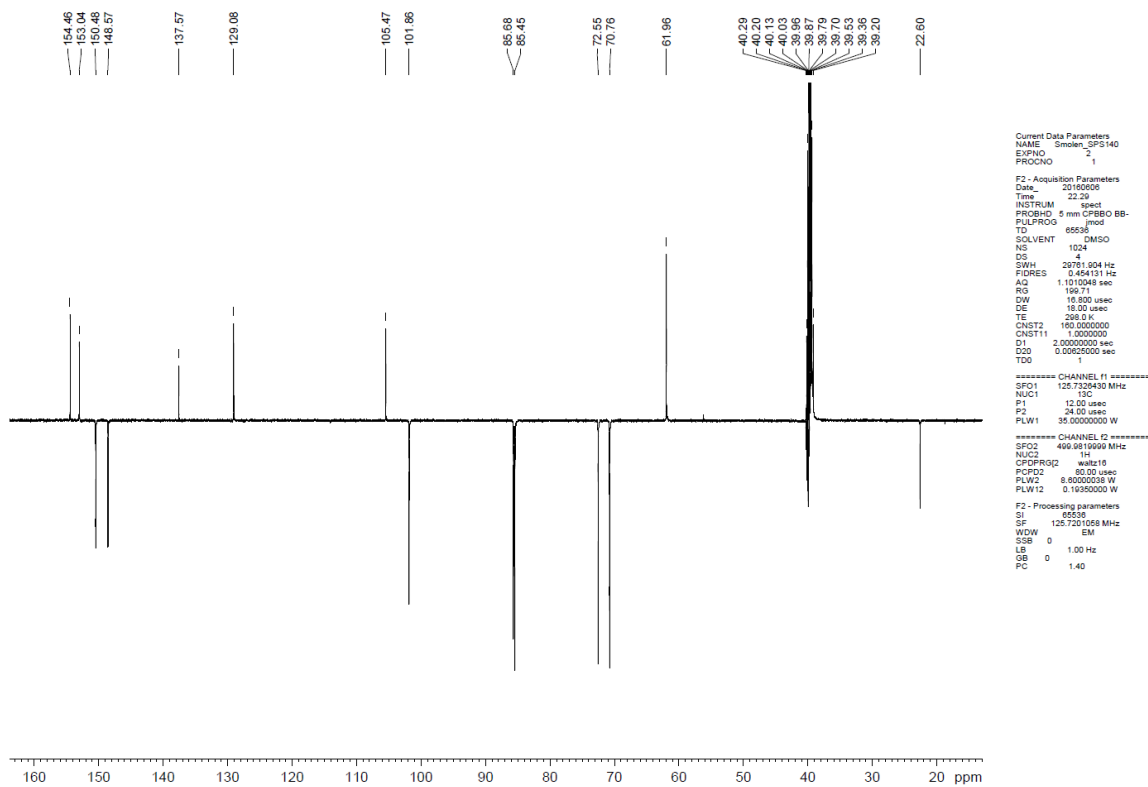
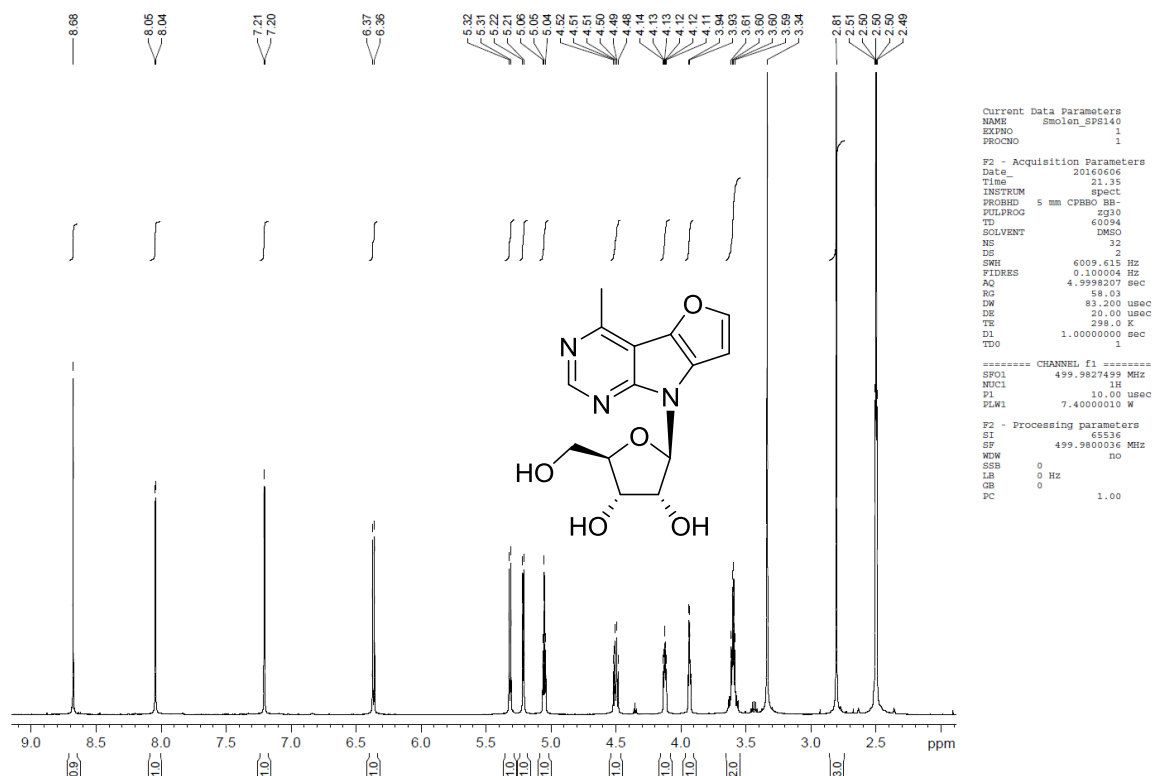
NMR spectra of compound **26b**



NMR spectra of compound **26c**

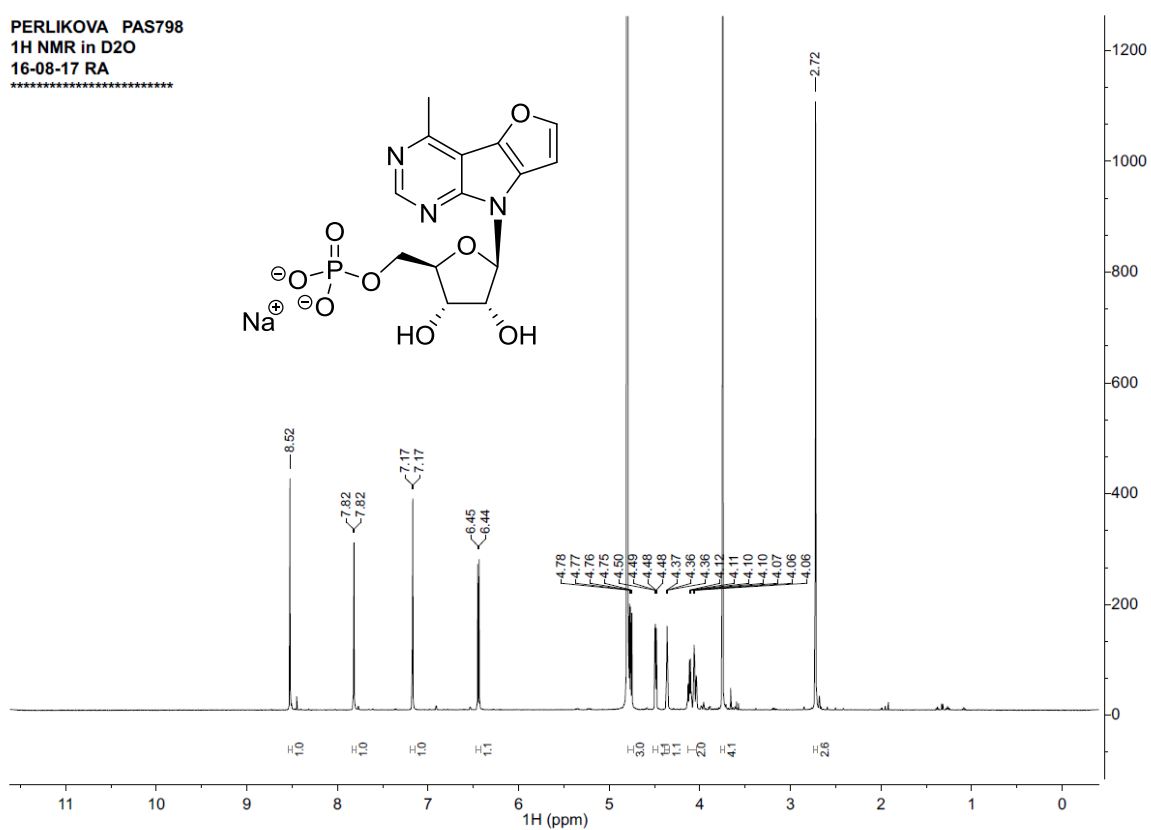


NMR spectra of compound **26d**

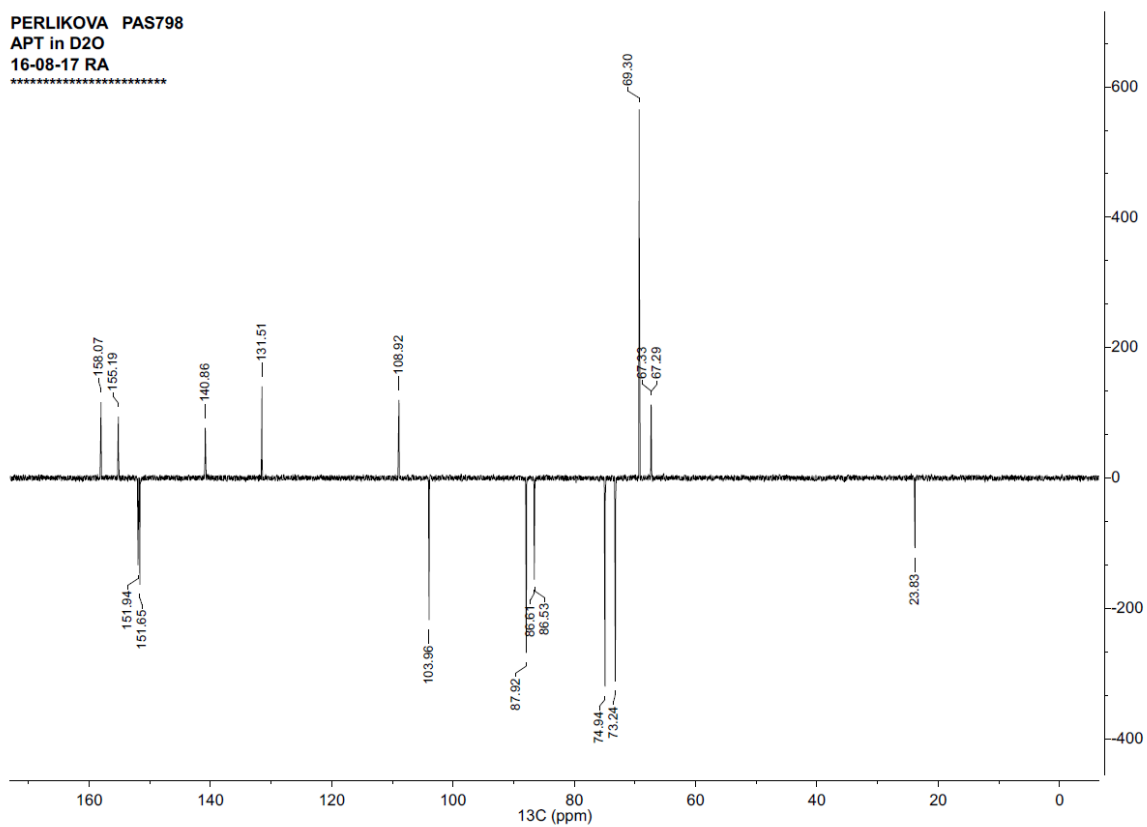


NMR spectra of compound **26d-MP**

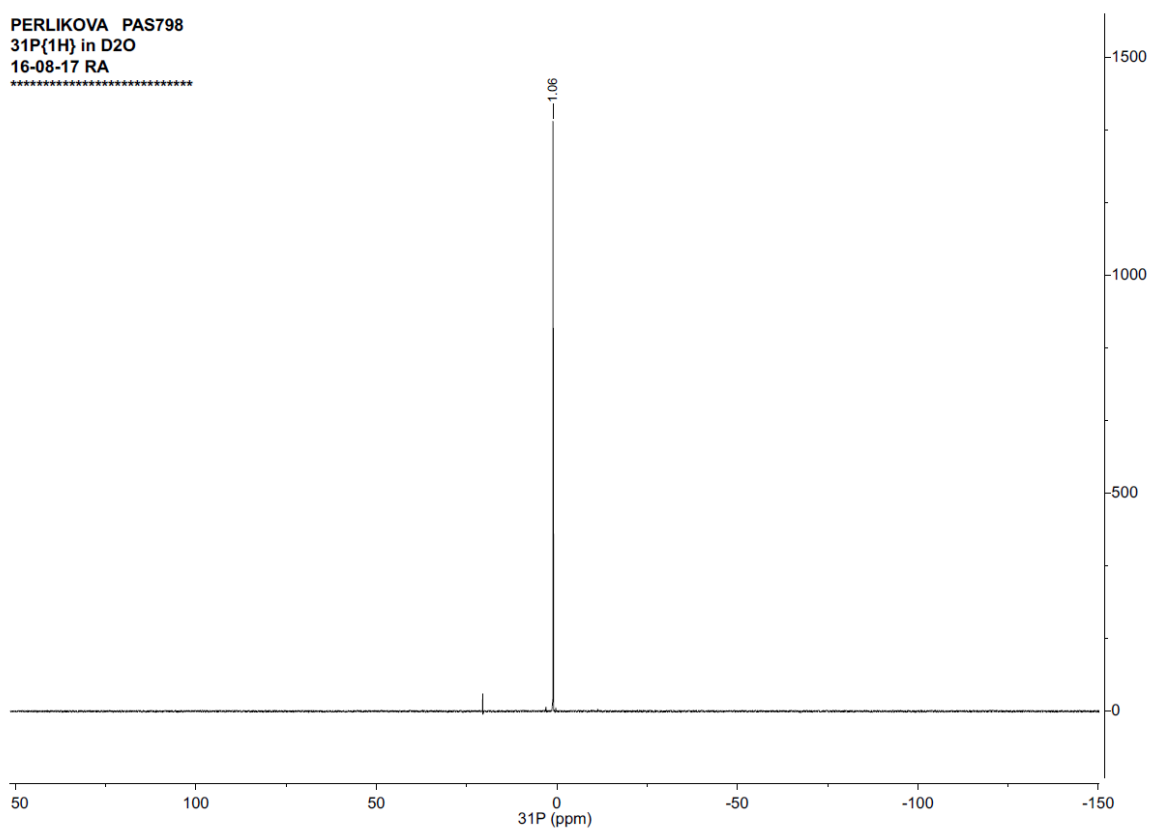
PERLIKOVA PAS798
1H NMR in D2O
16-08-17 RA



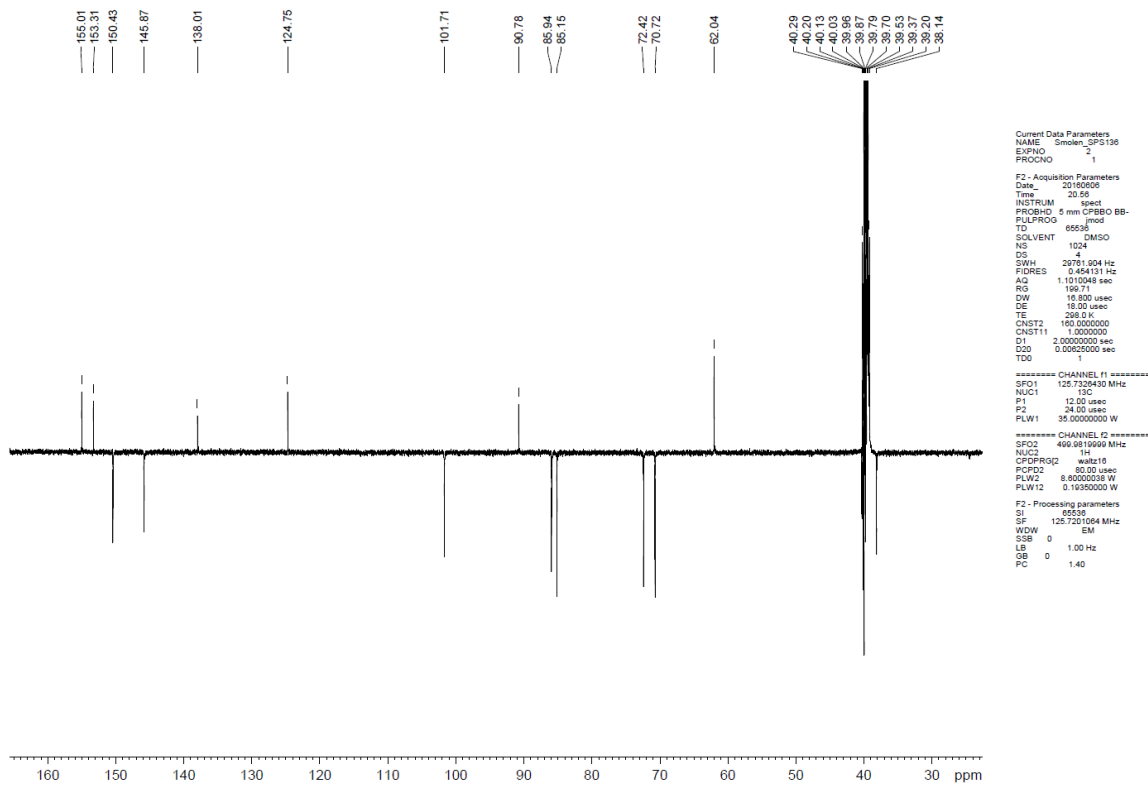
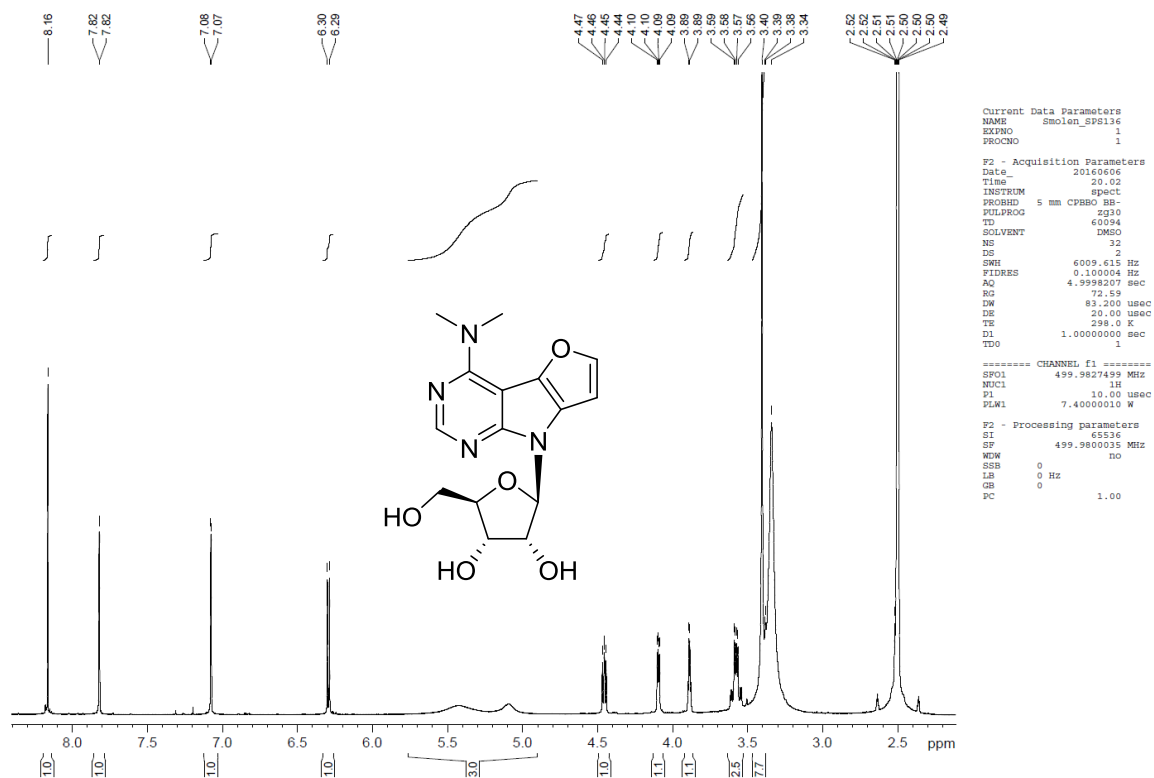
PERLIKOVA PAS798
APT in D2O
16-08-17 RA



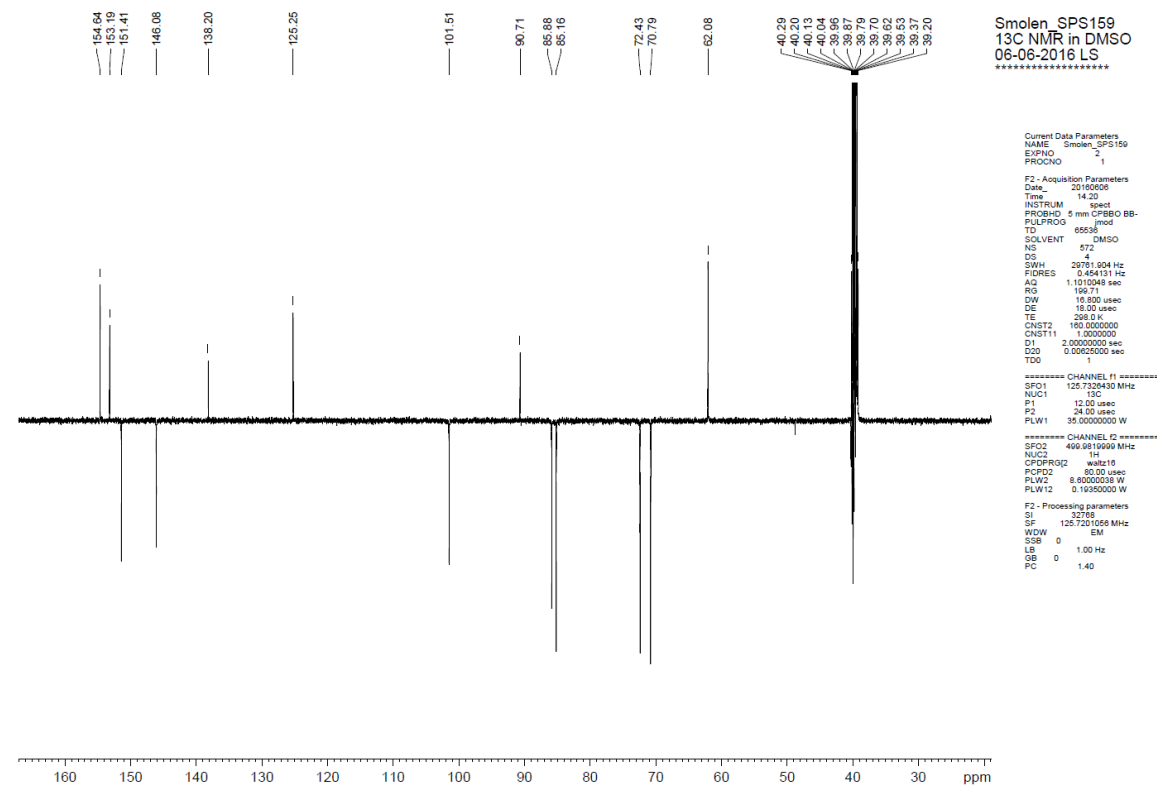
PERLIKOVA PAS798
31P{1H} in D2O
16-08-17 RA



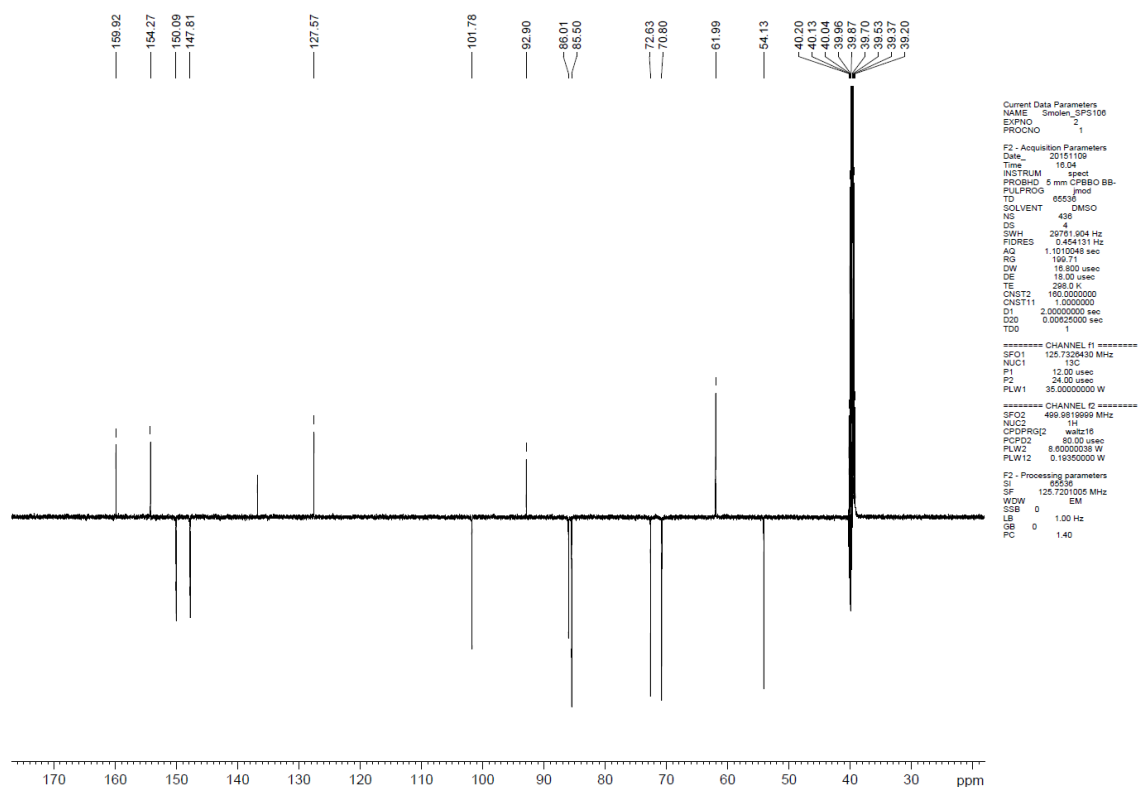
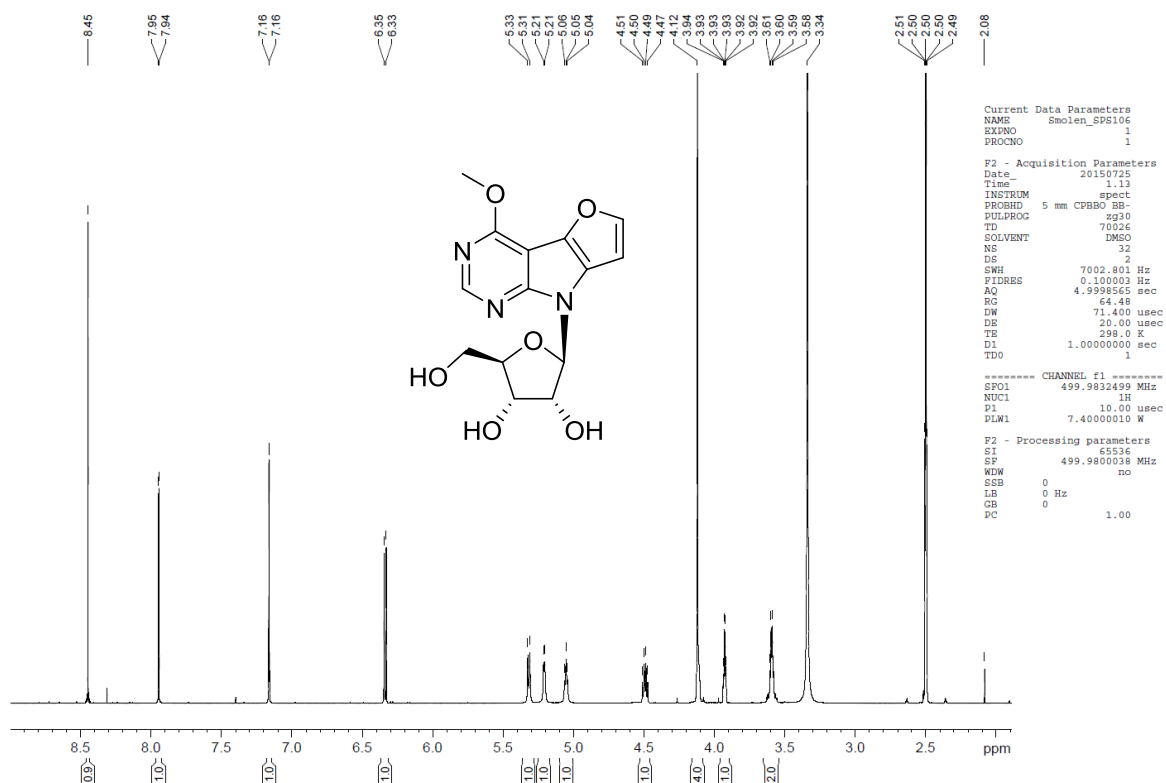
NMR spectra of compound **26e**



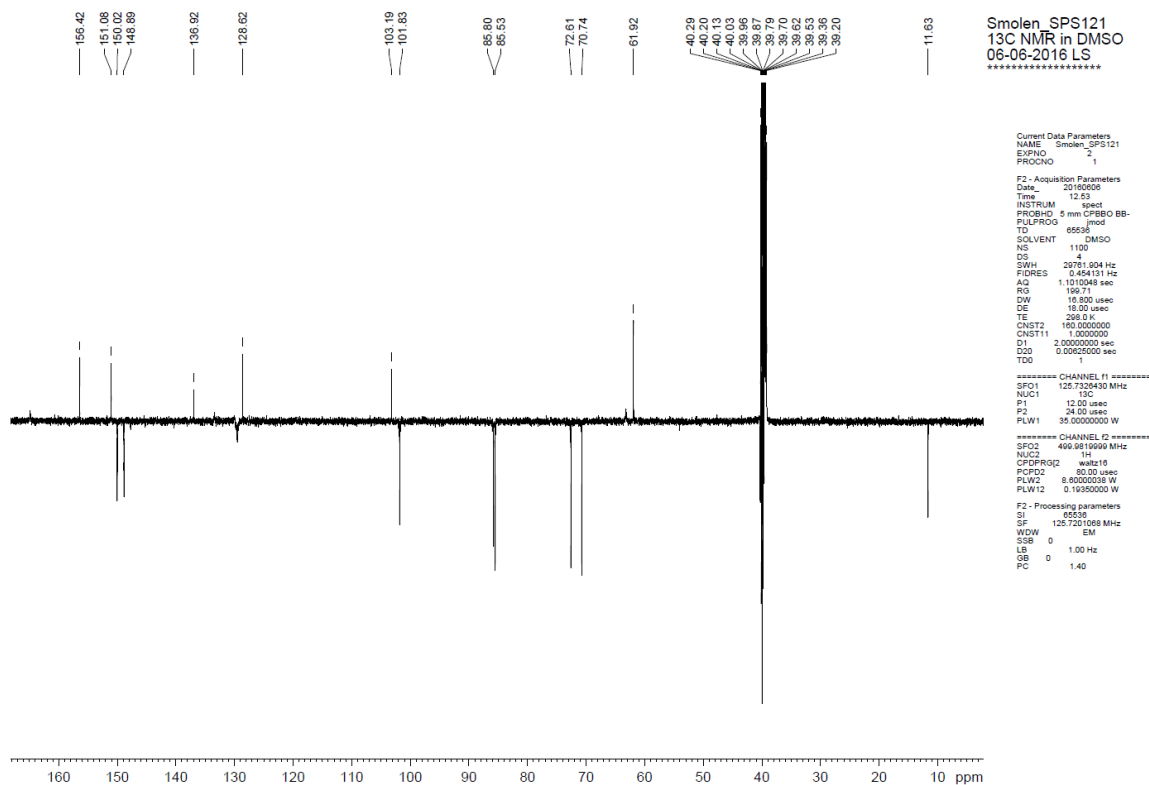
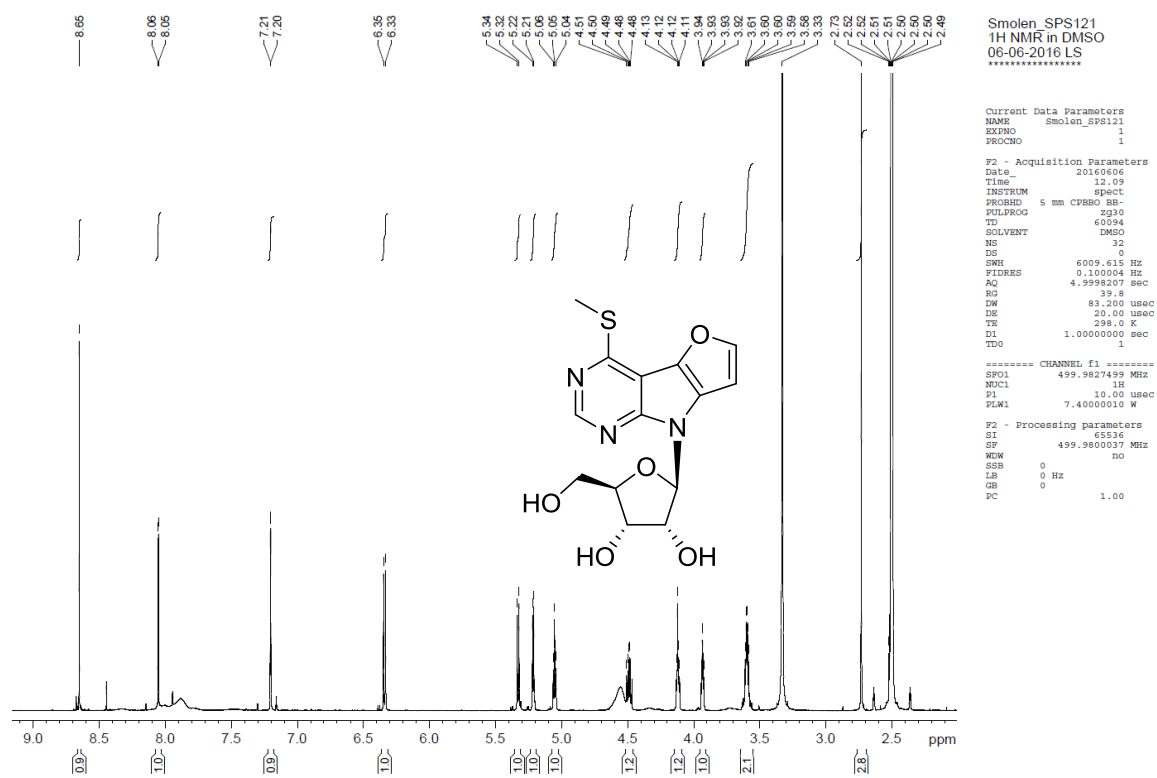
S63



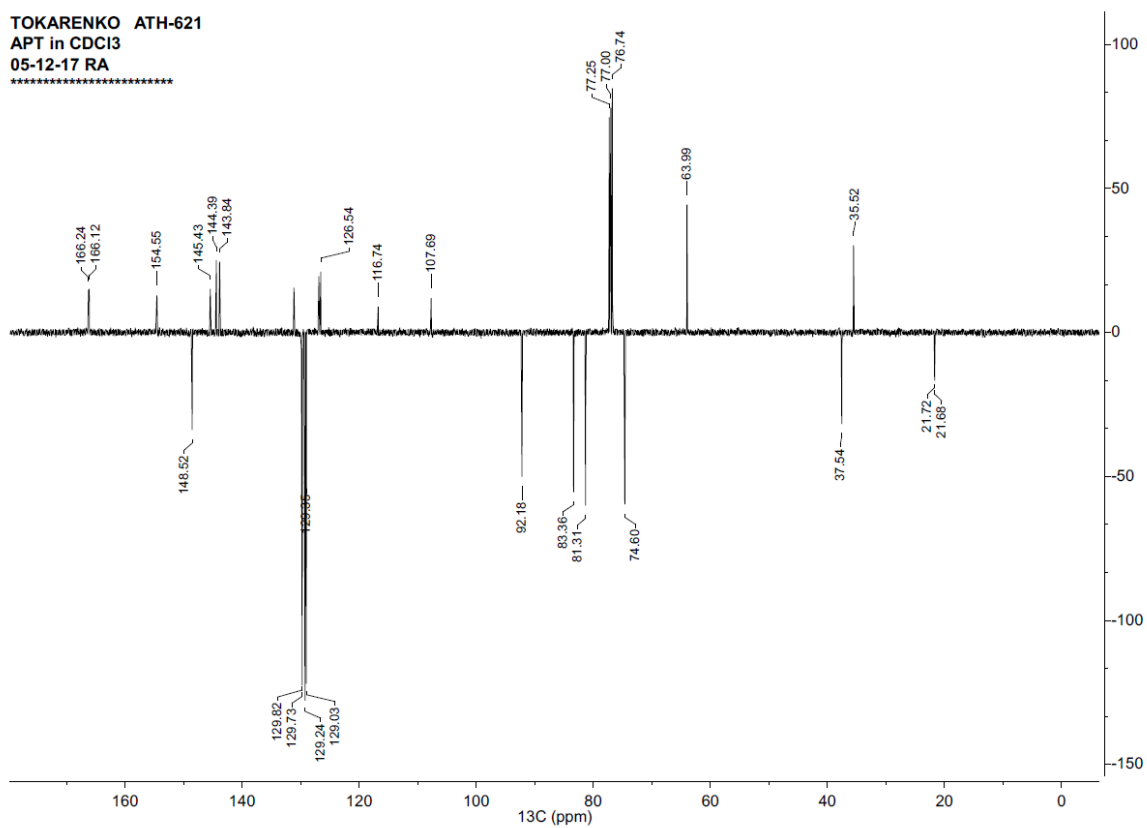
S64

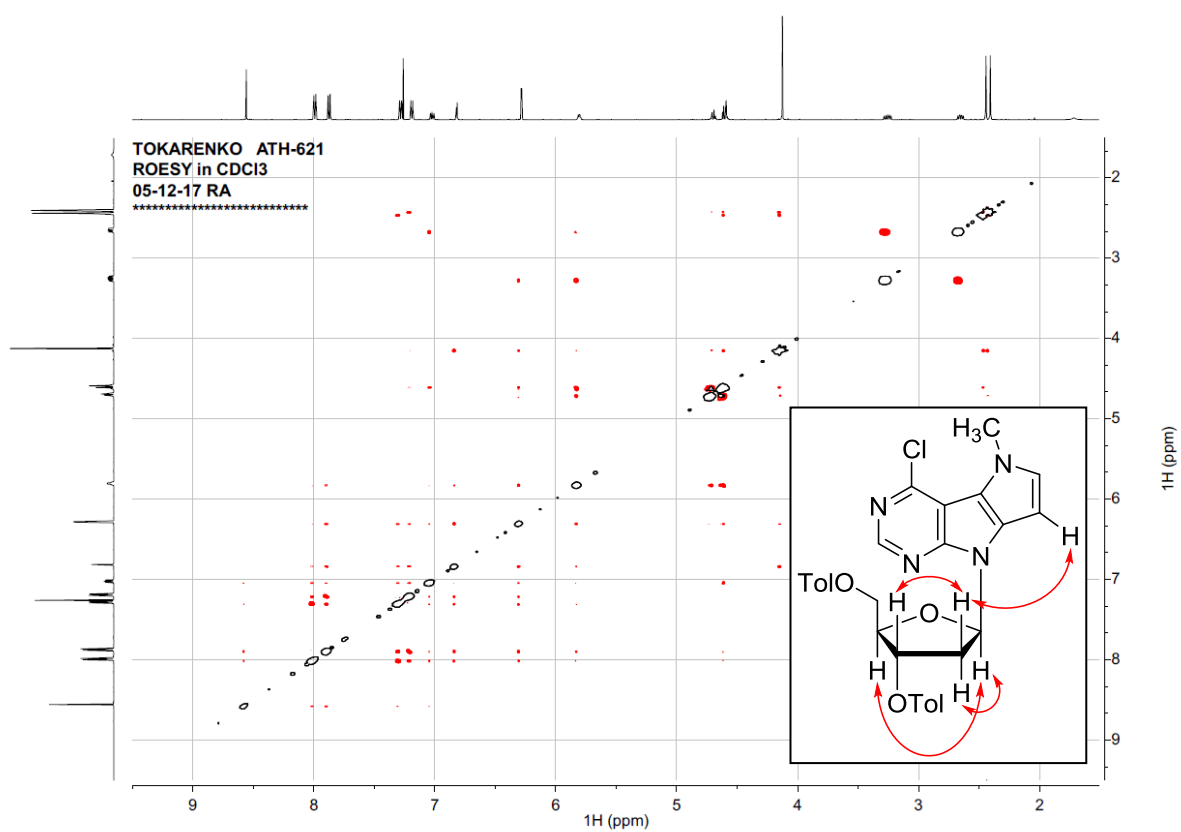


NMR spectra of compound **26h**

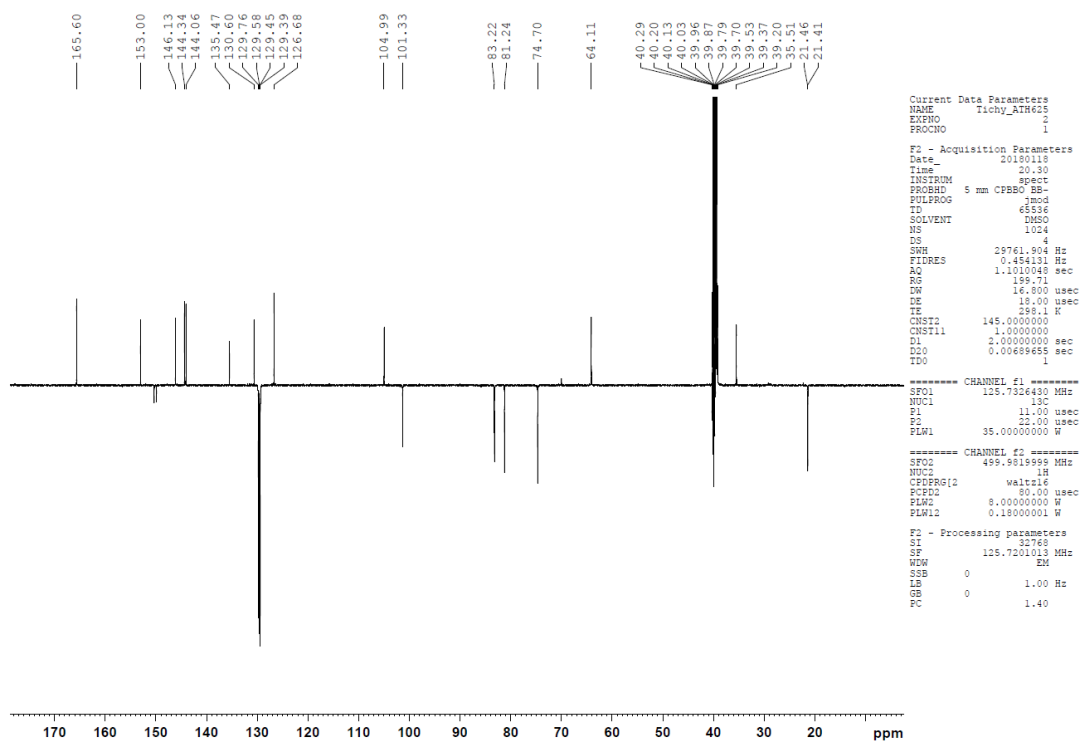
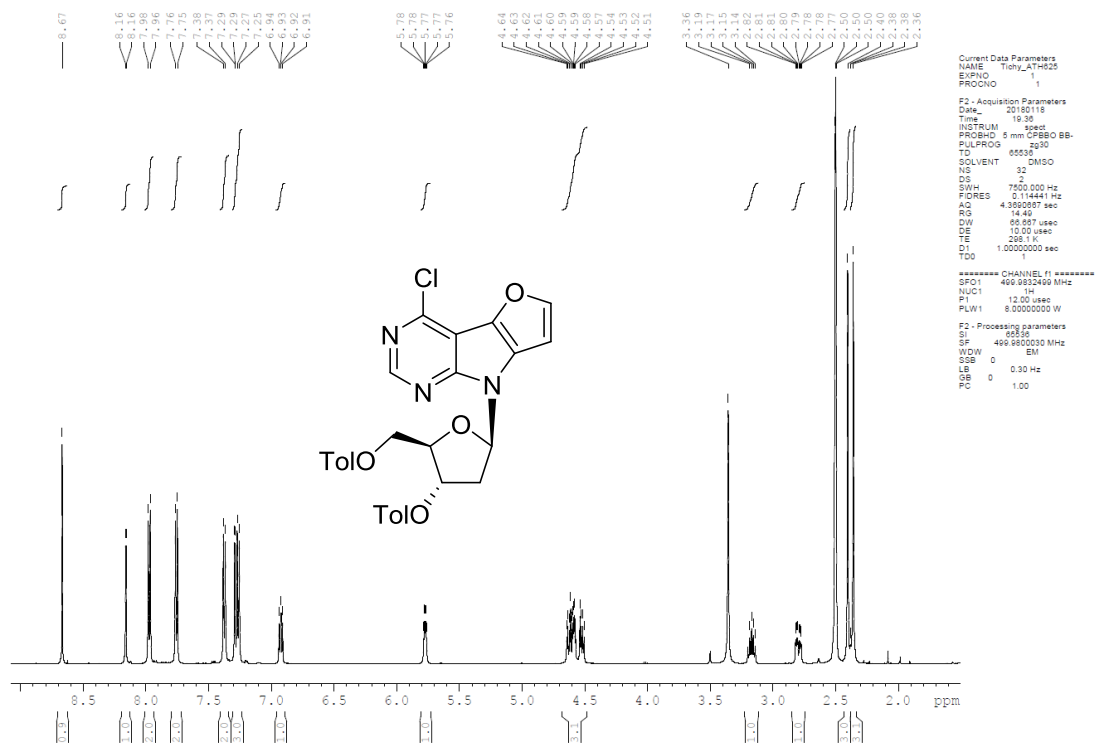


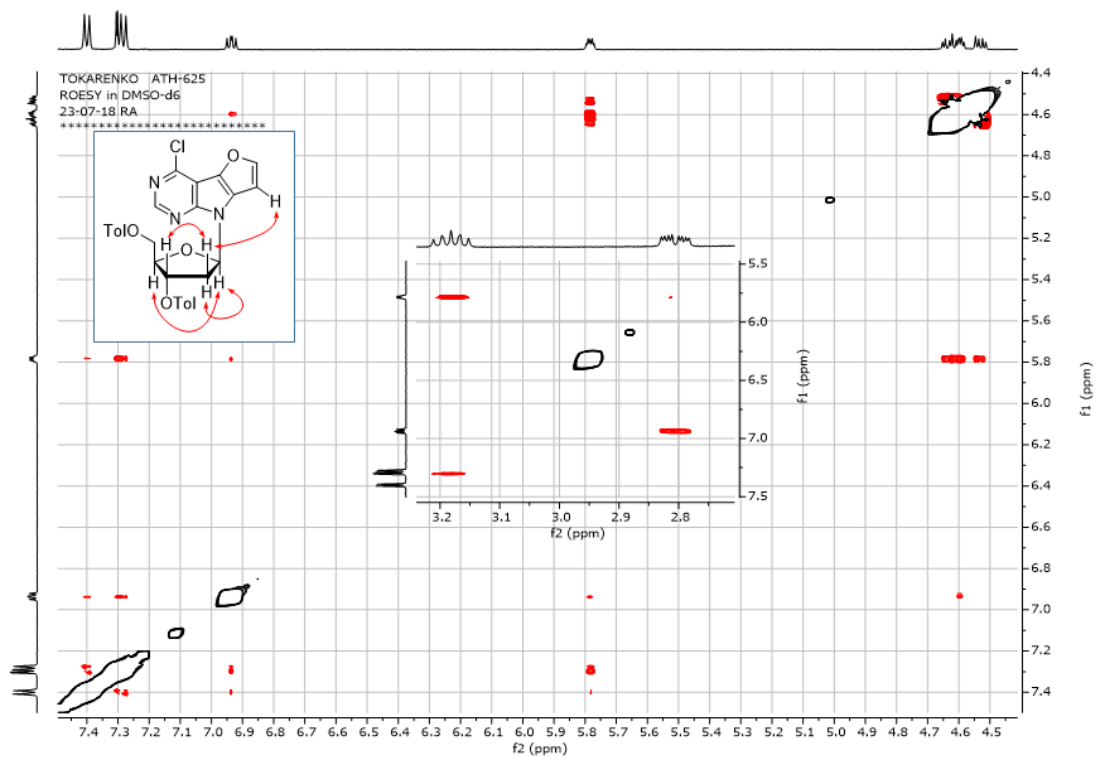
TOKARENKO ATH-621
1H NMR in CDCl3
05-12-17 RA



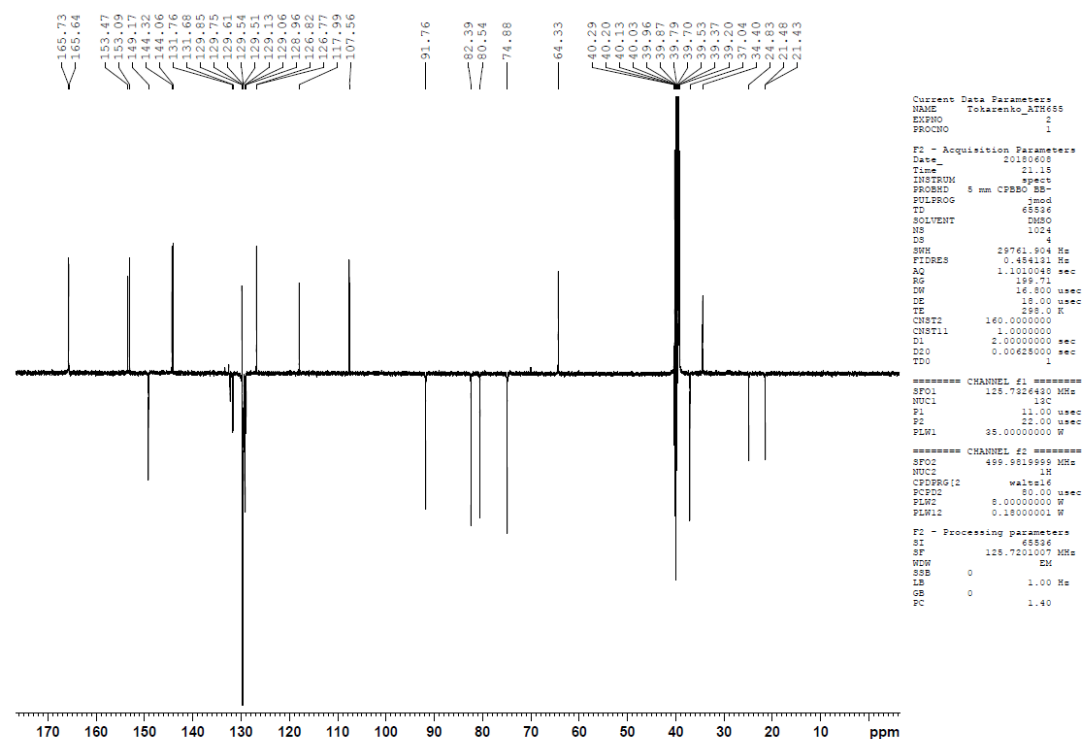
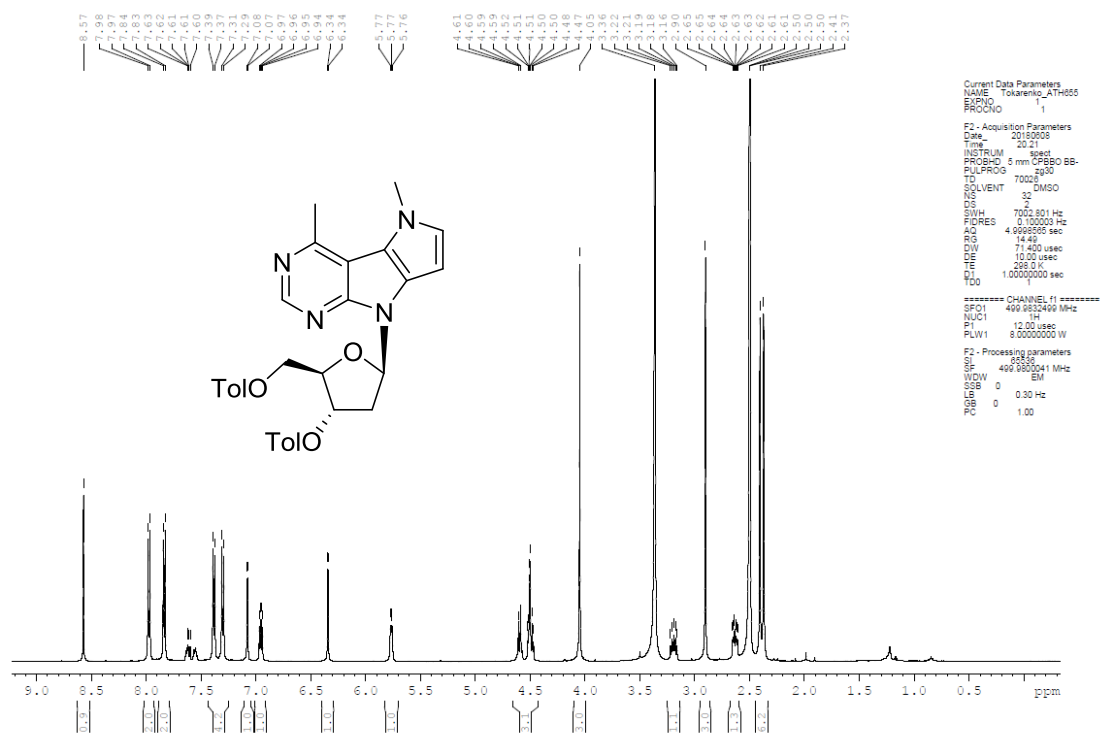


NMR spectra of compound **28**

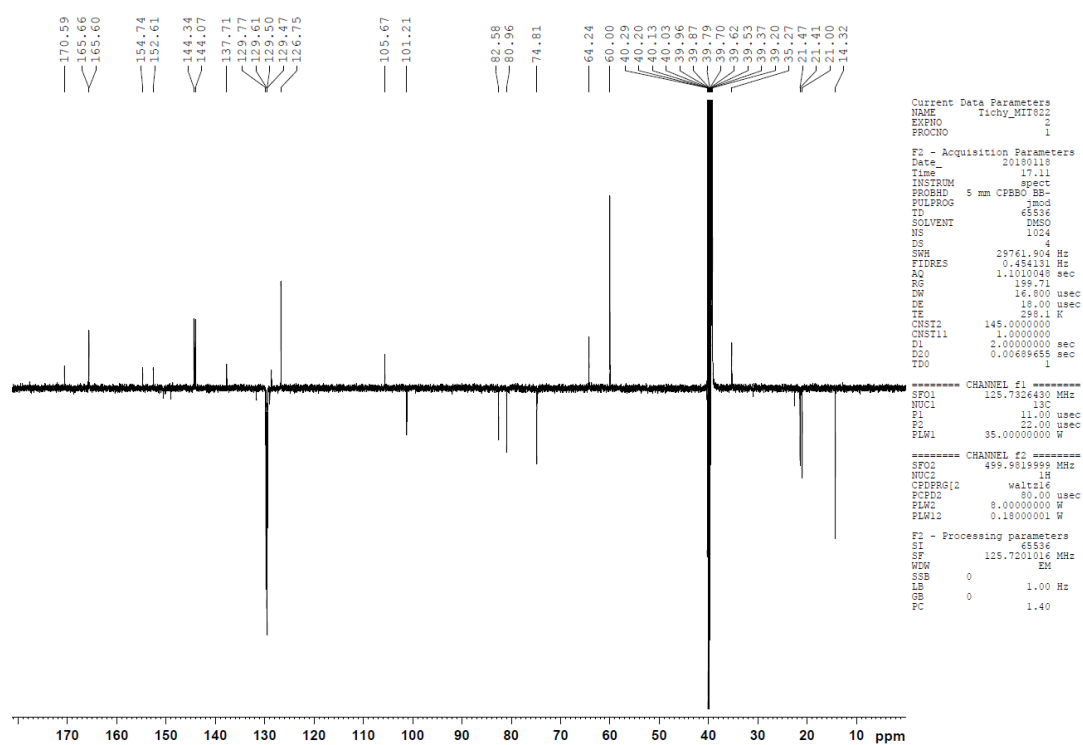
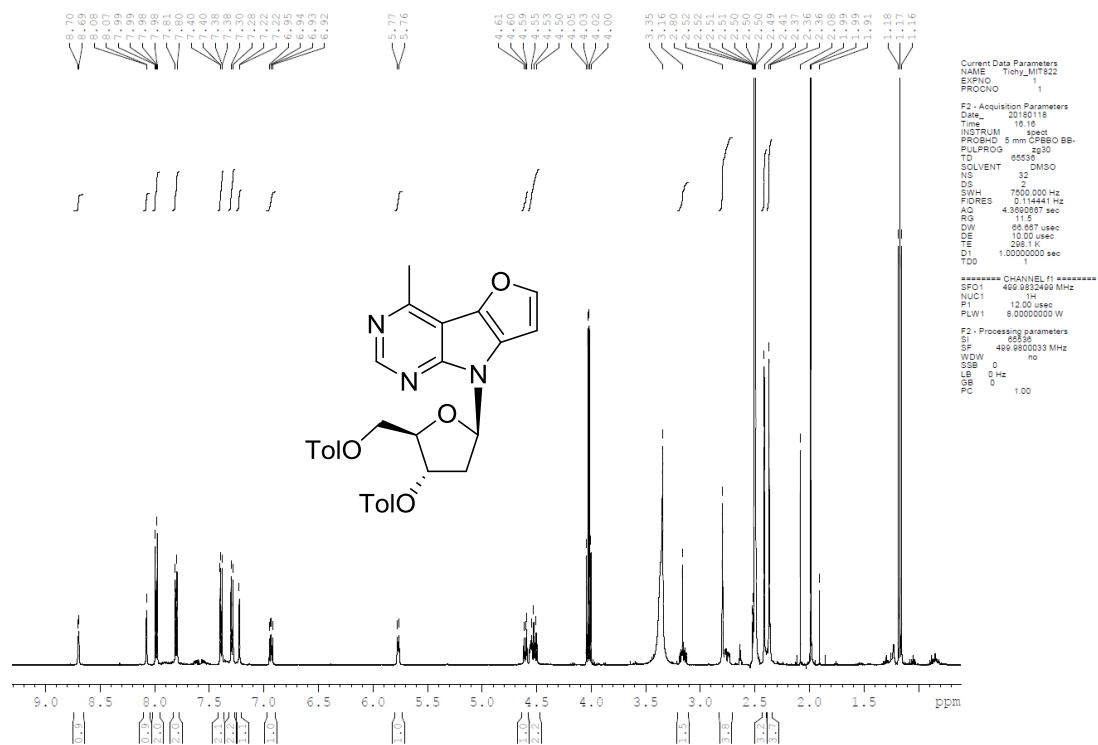




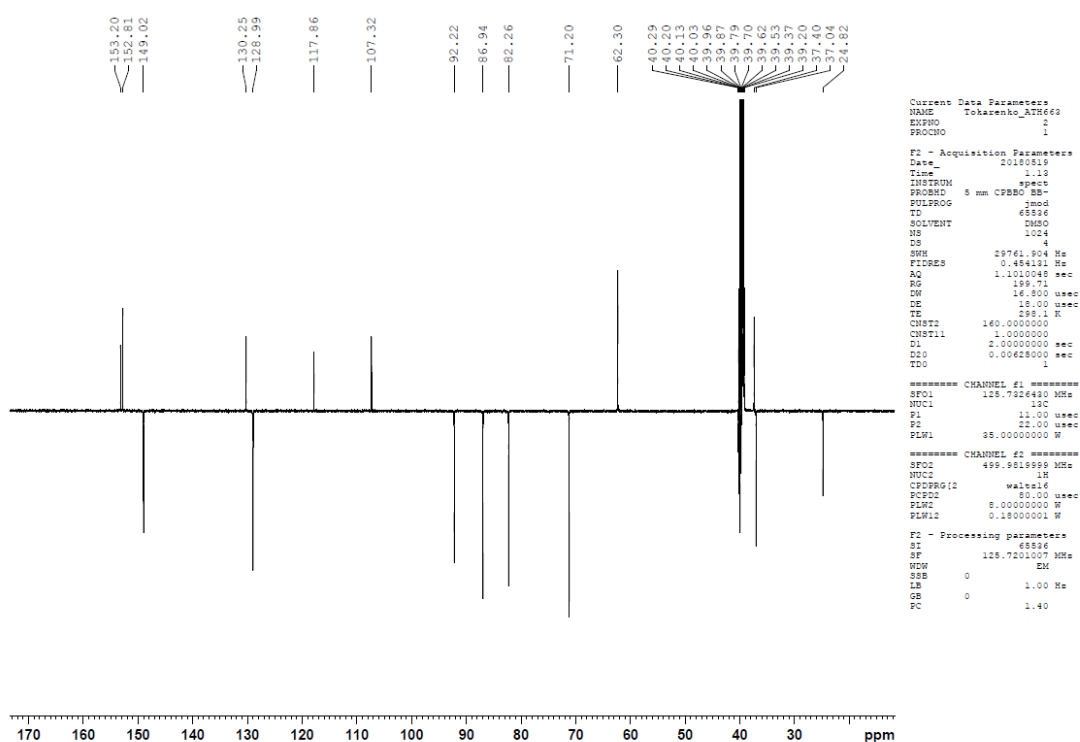
NMR spectra of compound **29**



NMR spectra of compound **30**



S72

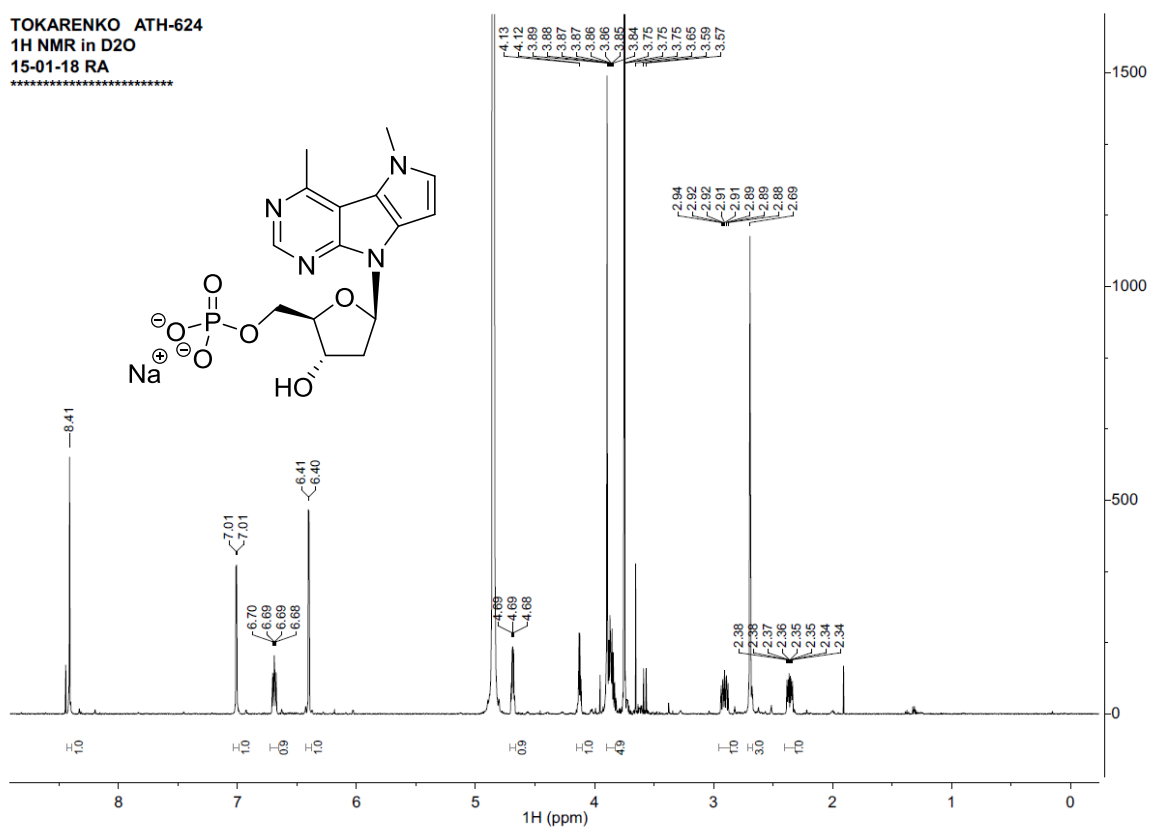


NMR spectra of compound **31-MP**

TOKARENKO ATH-624

¹H NMR in D₂O

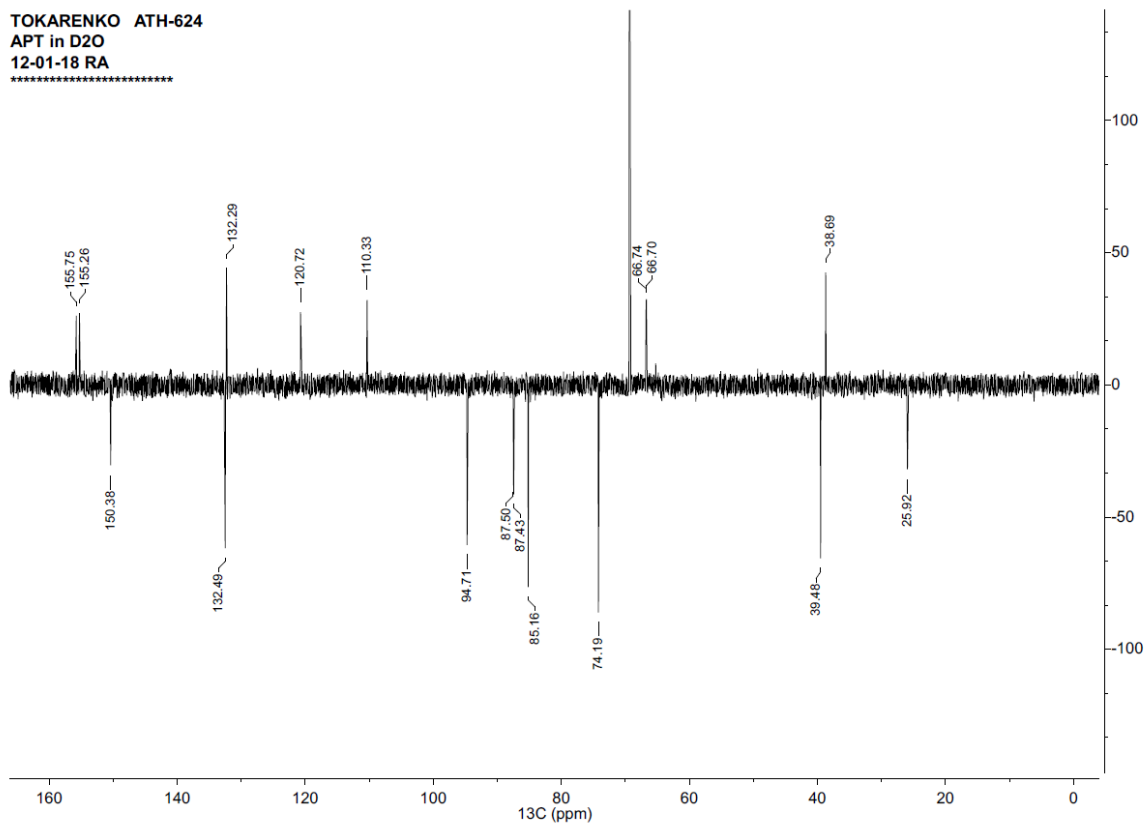
15-01-18 RA



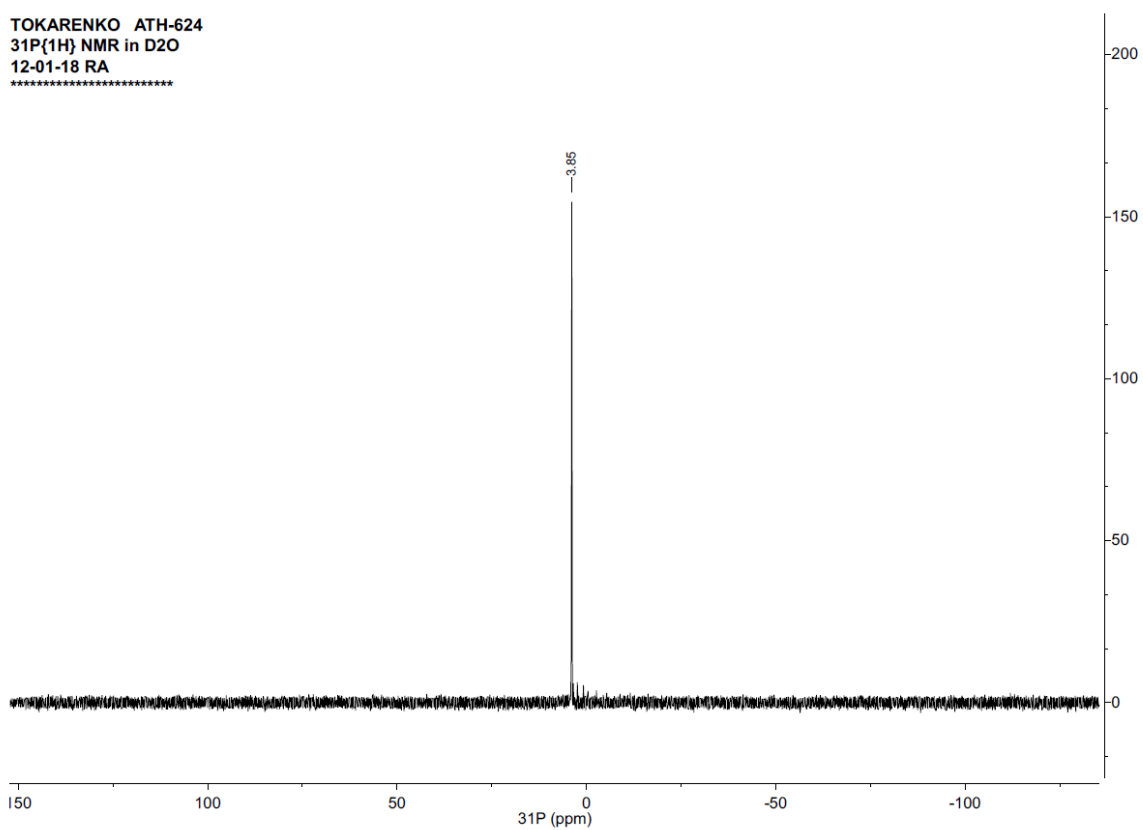
TOKARENKO ATH-624

APT in D₂O

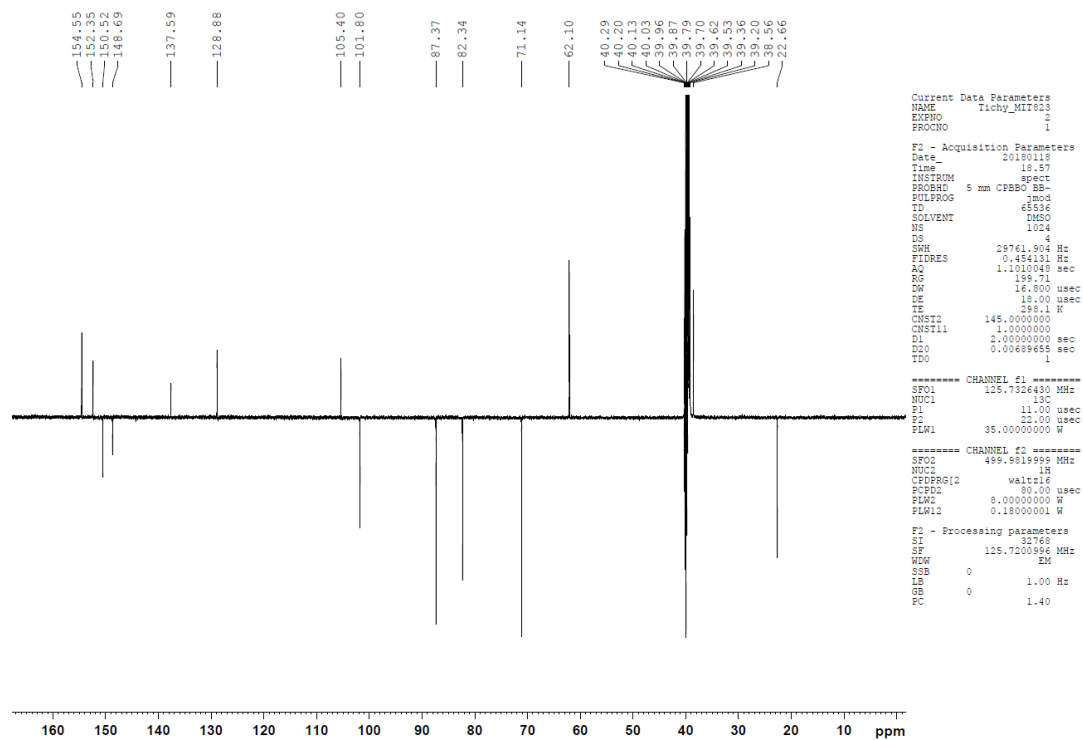
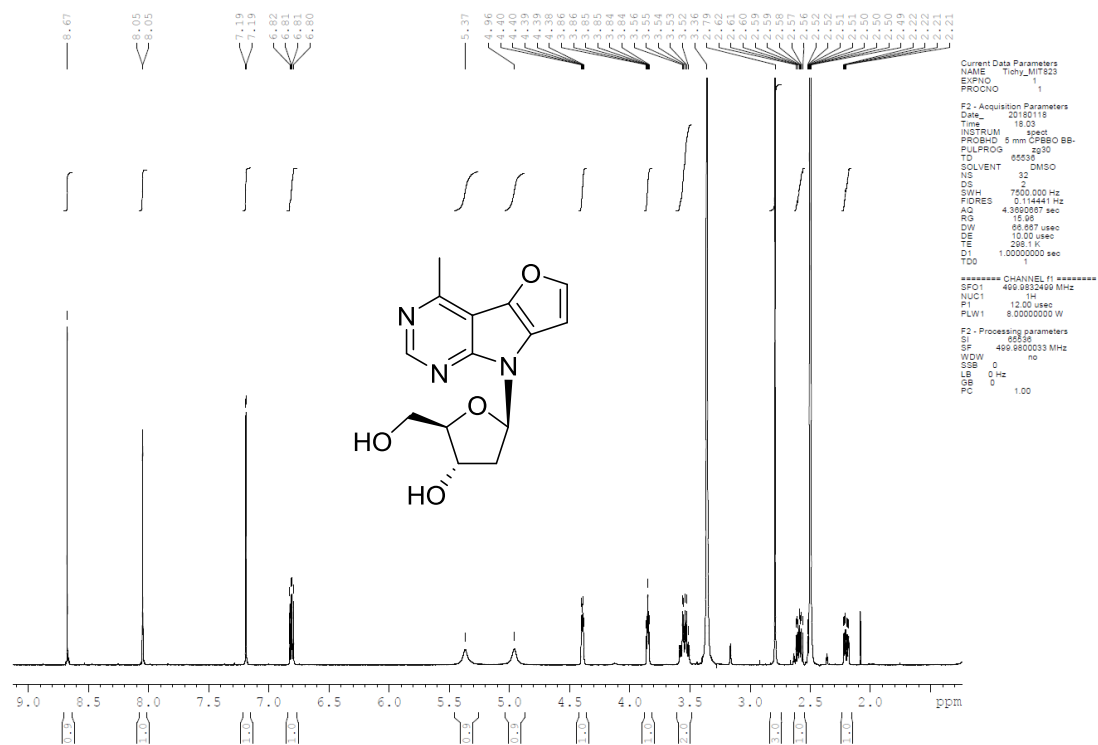
12-01-18 RA



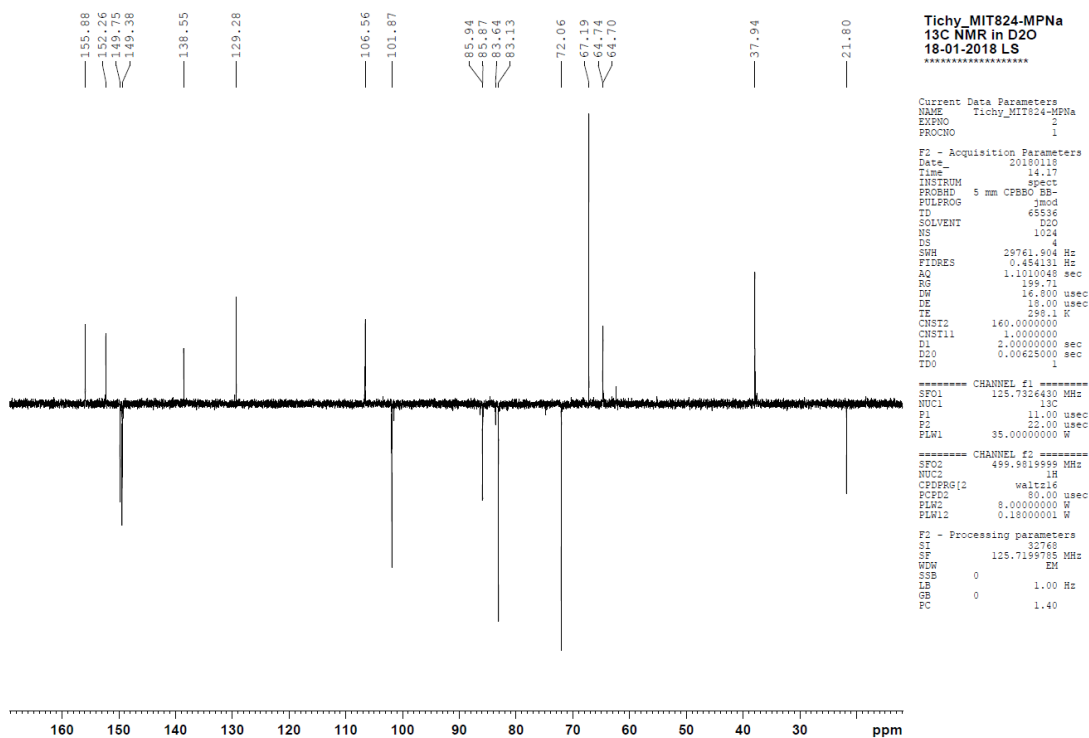
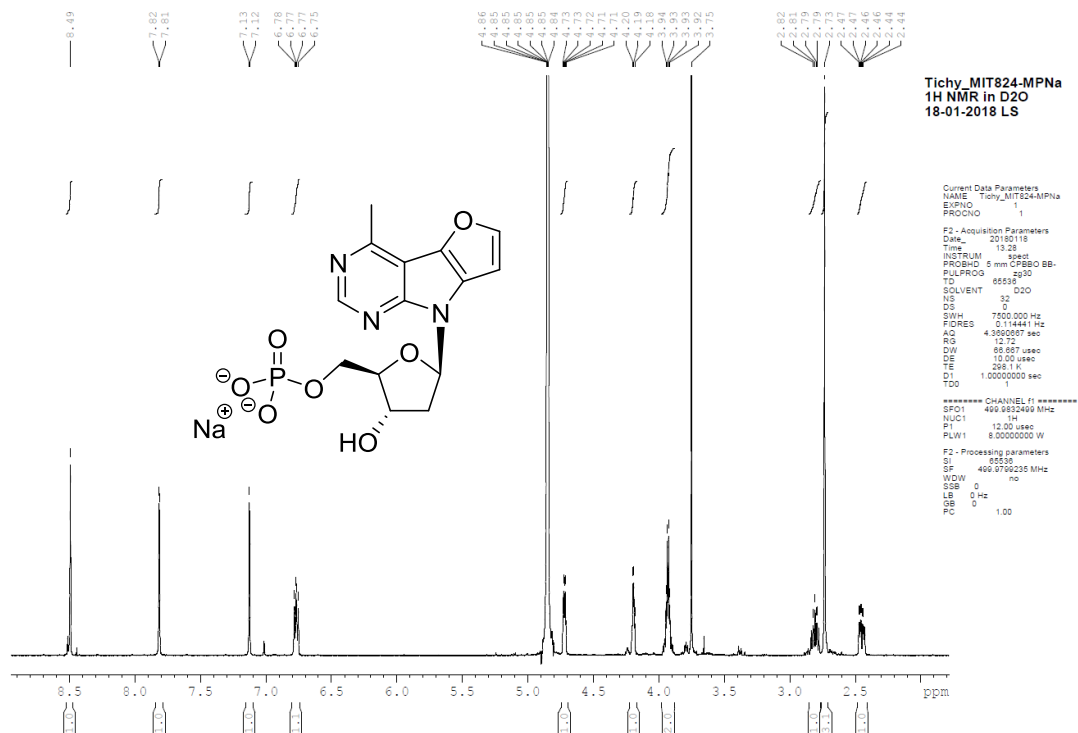
TOKARENKO ATH-624
31P{1H} NMR in D2O
12-01-18 RA

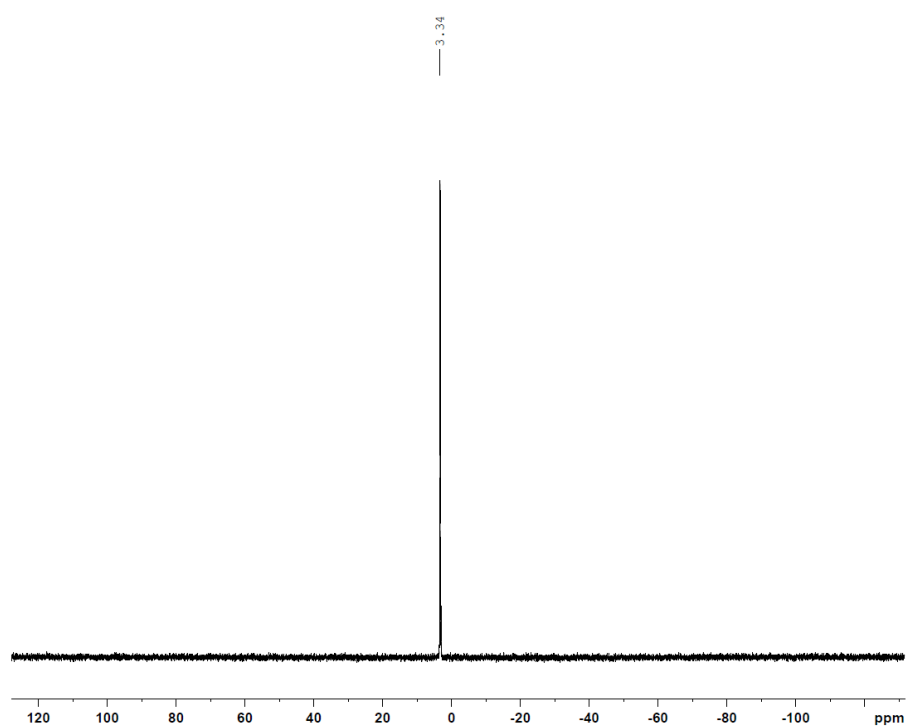


S75



NMR spectra of compound **32-MP**





Tichy_MIT824-MPNa
 31P(H) in D2O
 18-01-2018 LS

Current Data Parameters
 NAME Tichy_MIT824-MPNa
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180118
 Time_ 15.22
 INSTRUM spect
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 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 32
 DS 0
 SWH 81521.742 Hz
 FIDRES 1.248923 Hz
 AQ 0.4018641 sec
 RG 199.71
 DW 6.133 usec
 DE 23.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 202.3854942 MHz
 NUC1 31P
 P1 12.00 usec
 PLW1 29.00000000 W

===== CHANNEL f2 =====
 SFO2 499.9815659 MHz
 NUC2 1H
 CPDPRG2 waltz16
 P1P2 89.00 usec
 PLW2 7.40000010 W
 PLW12 0.13991000 W
 PLW13 0.07037200 W

F2 - Processing parameters
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 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40