

Hexafluoroisopropanol mediated benign synthesis of 2H-pyrido[1,2-a]pyrimidin-2-ones by using a domino protocol

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Mohammad A Alam

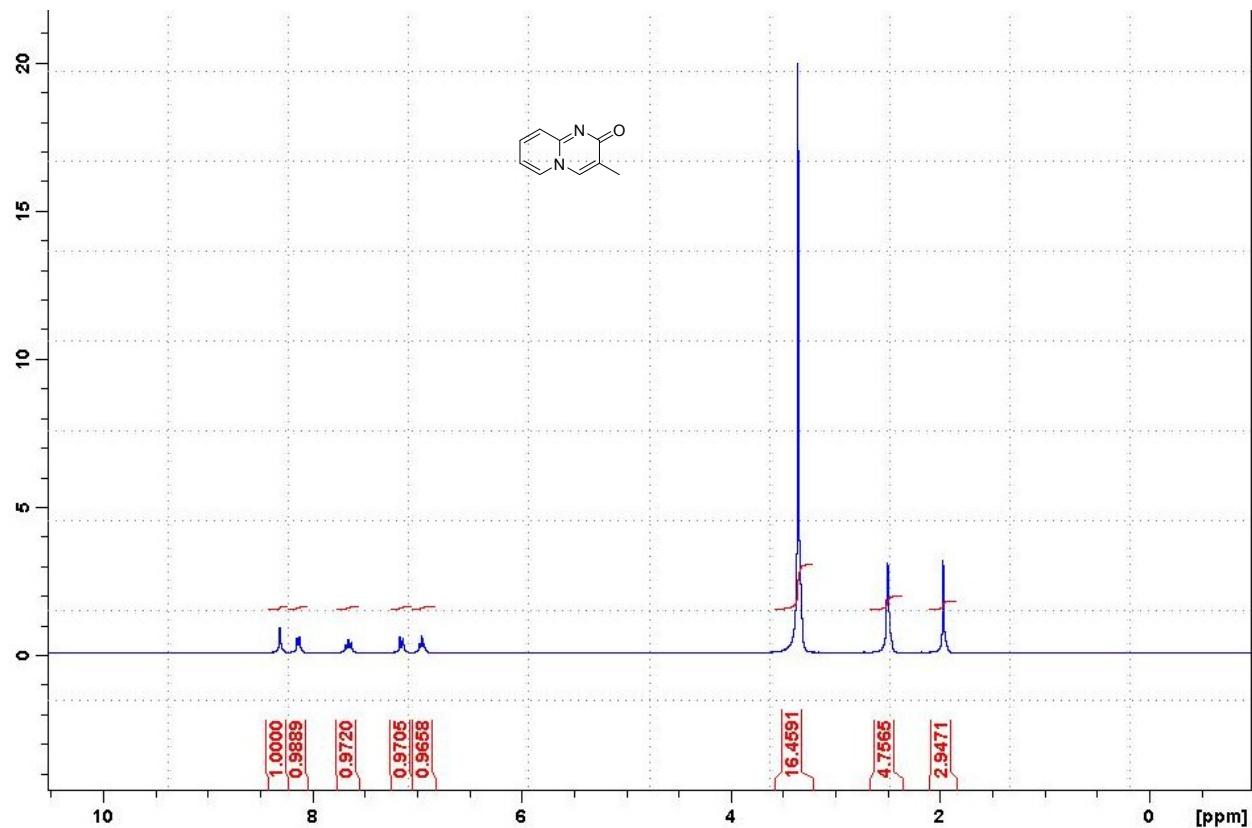
E-mail: malam@astate.edu, Tel: +1-870-973-3319

Materials and instrumentation

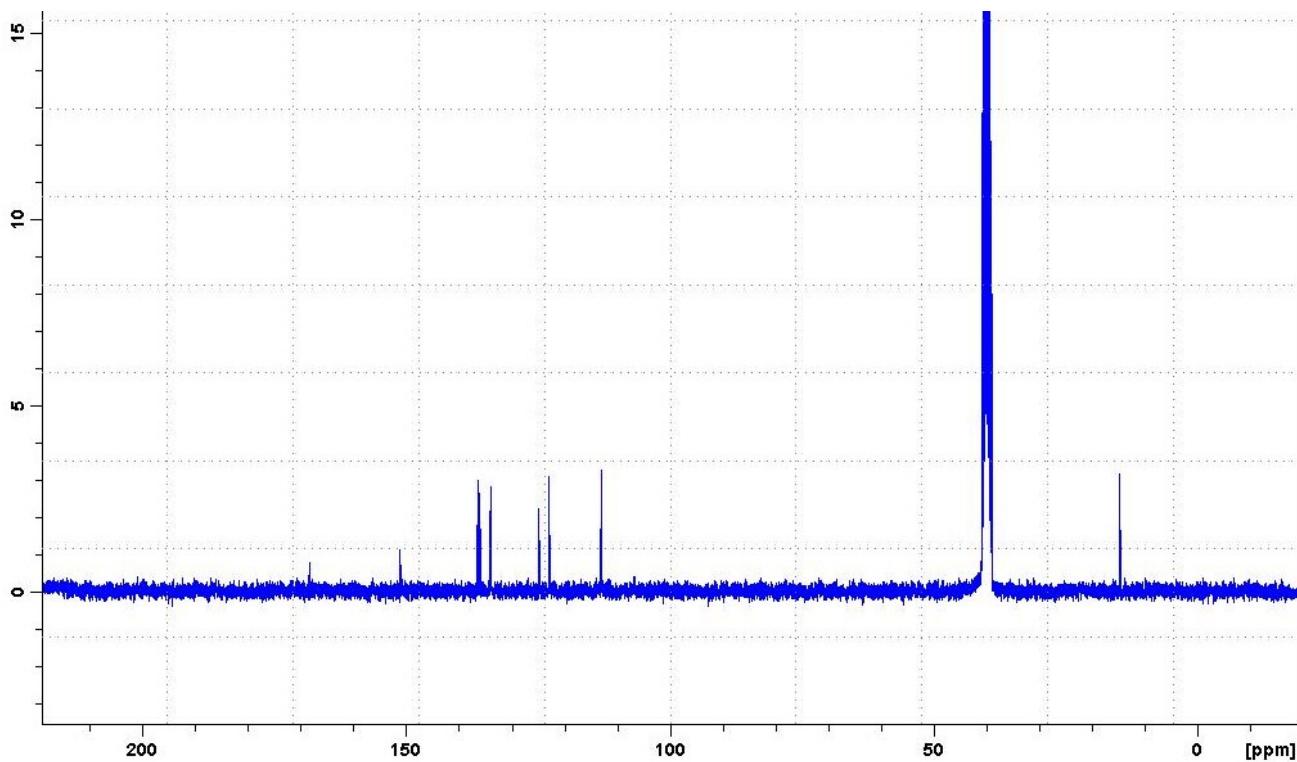
All commercial chemicals and solvents are reagent grade and were used without further treatment unless otherwise noted. ¹H NMR spectra were obtained with a Varian Mercury-300MHz with TMS as internal standard. ¹³C NMR spectra were obtained with a Varian Mercury-75MHz with TMS as internal standard. The ESI-FTMS Mass spectra were recorded Bruker ApexII-FTMS system. Low resolution mass spectra were recorded in Shimadzu QQQ instrument.

3-Methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (12)

¹H NMR of 12

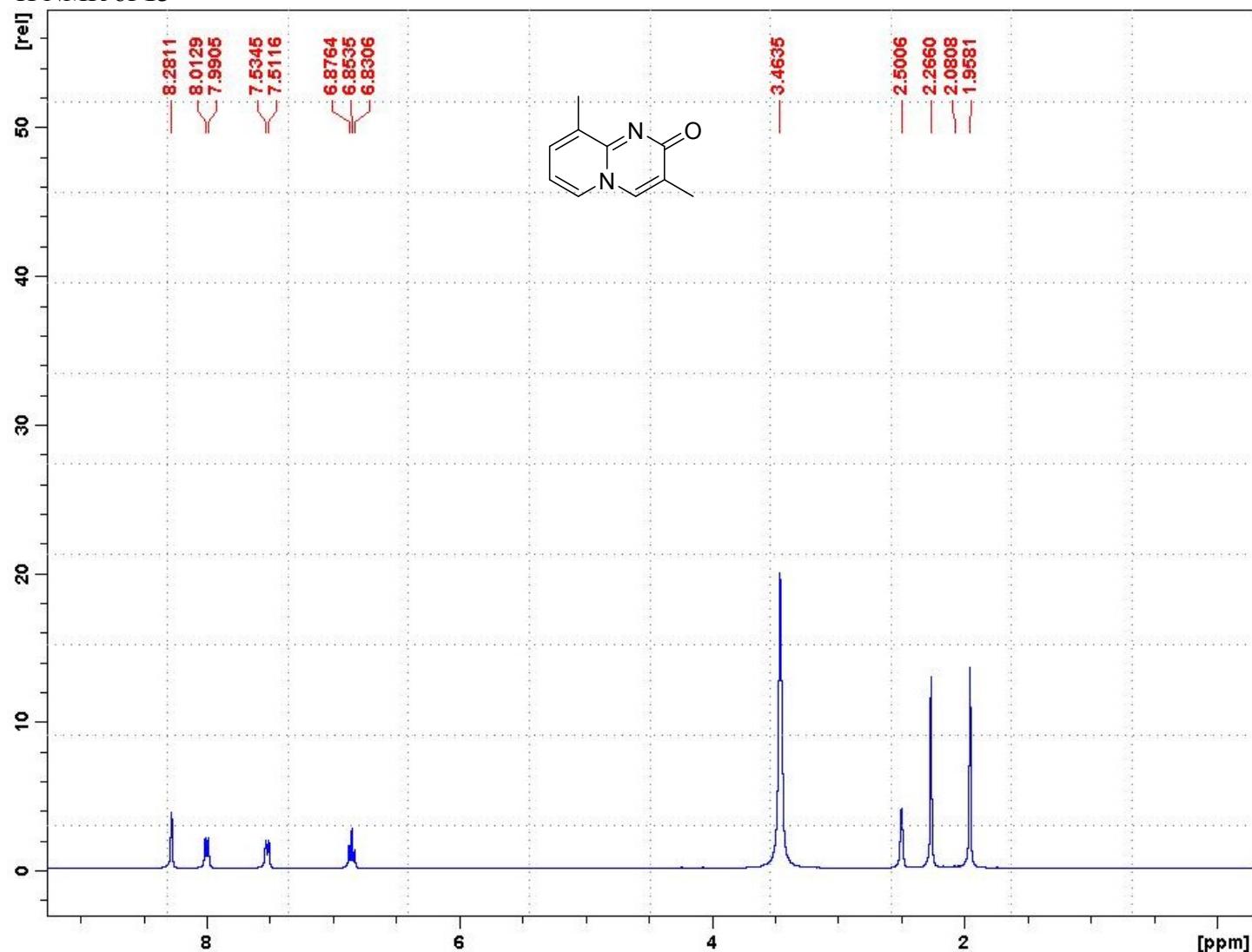


¹³C NMR of 12

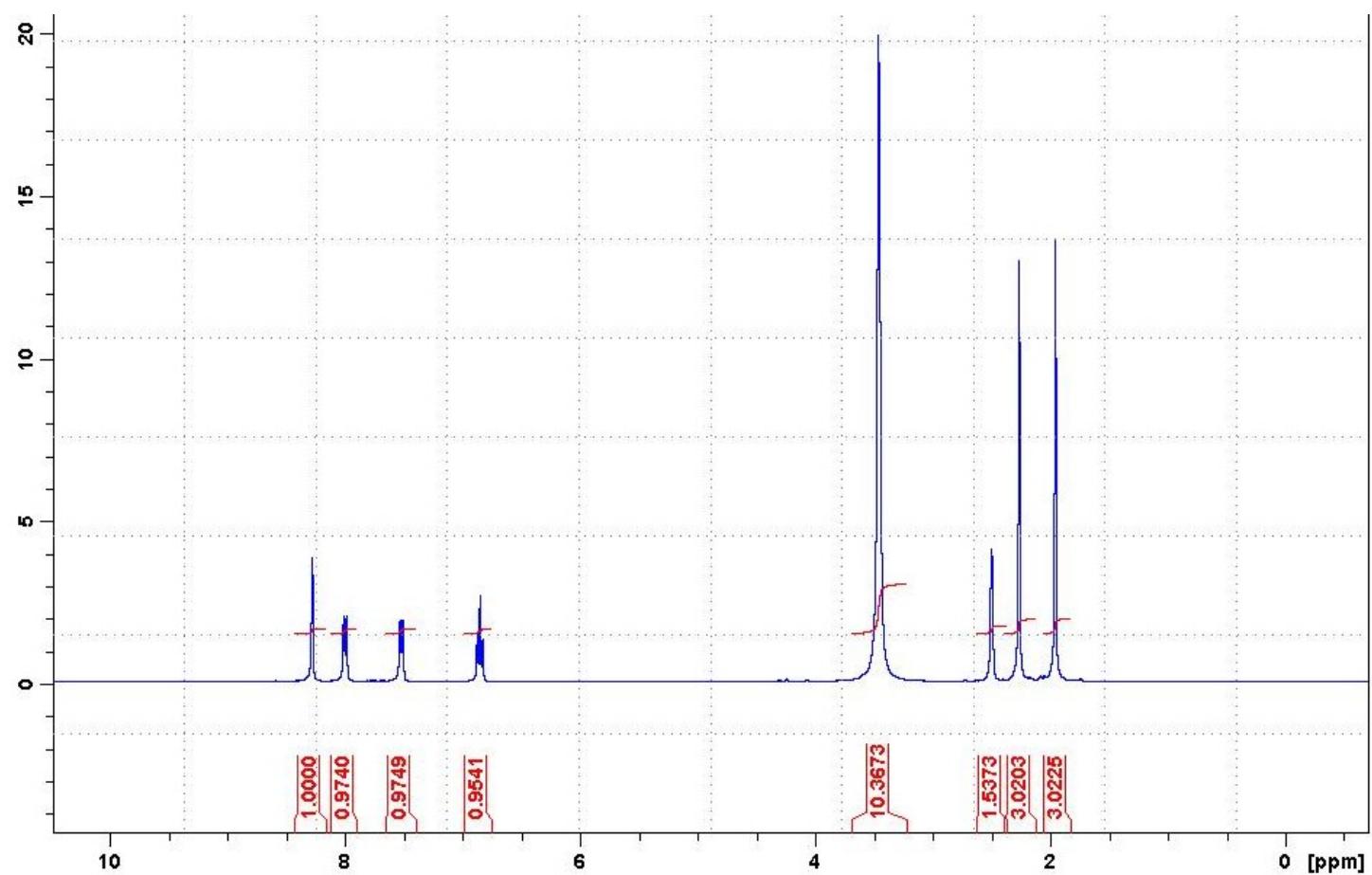


3,9-Dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (13)

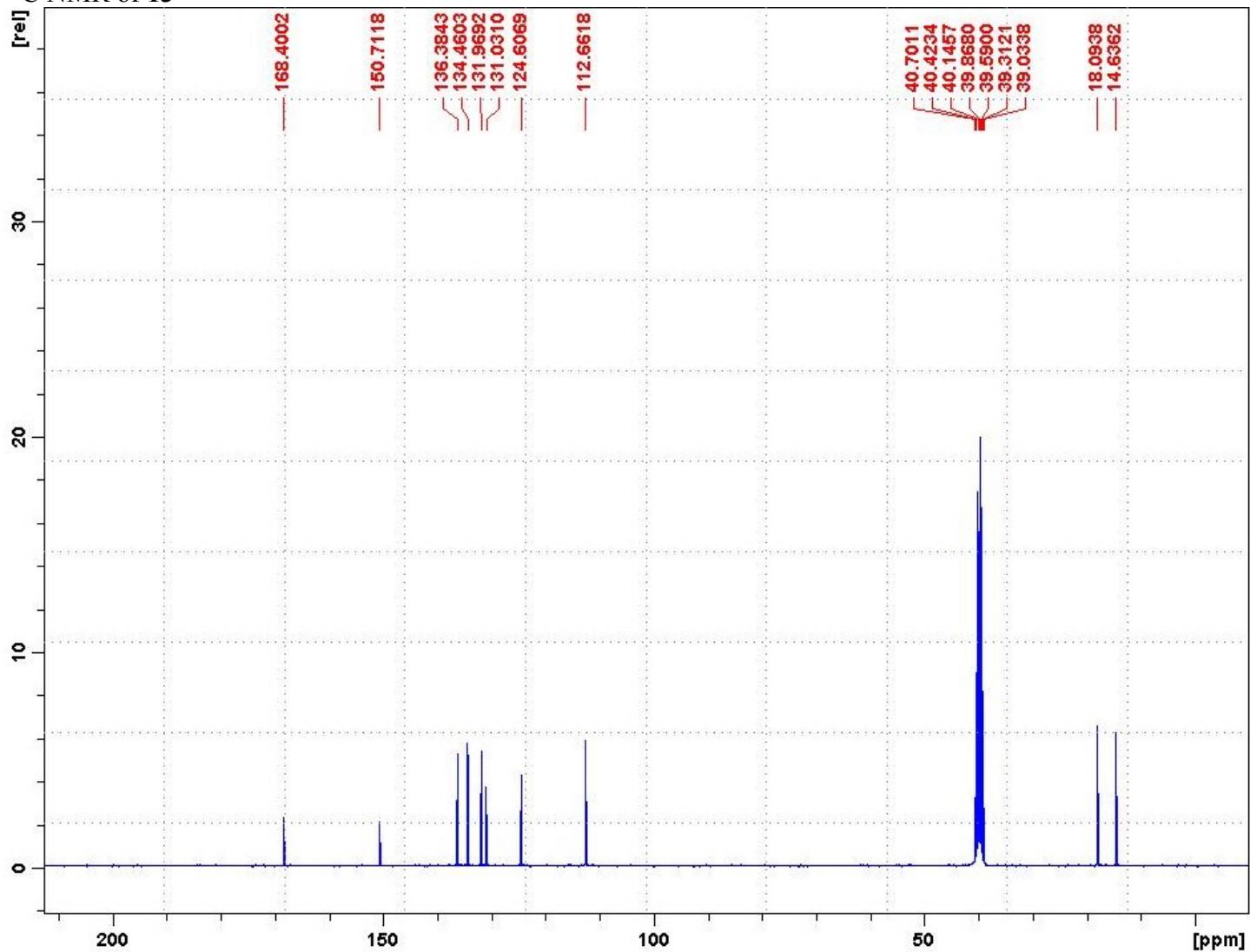
¹H NMR of 13



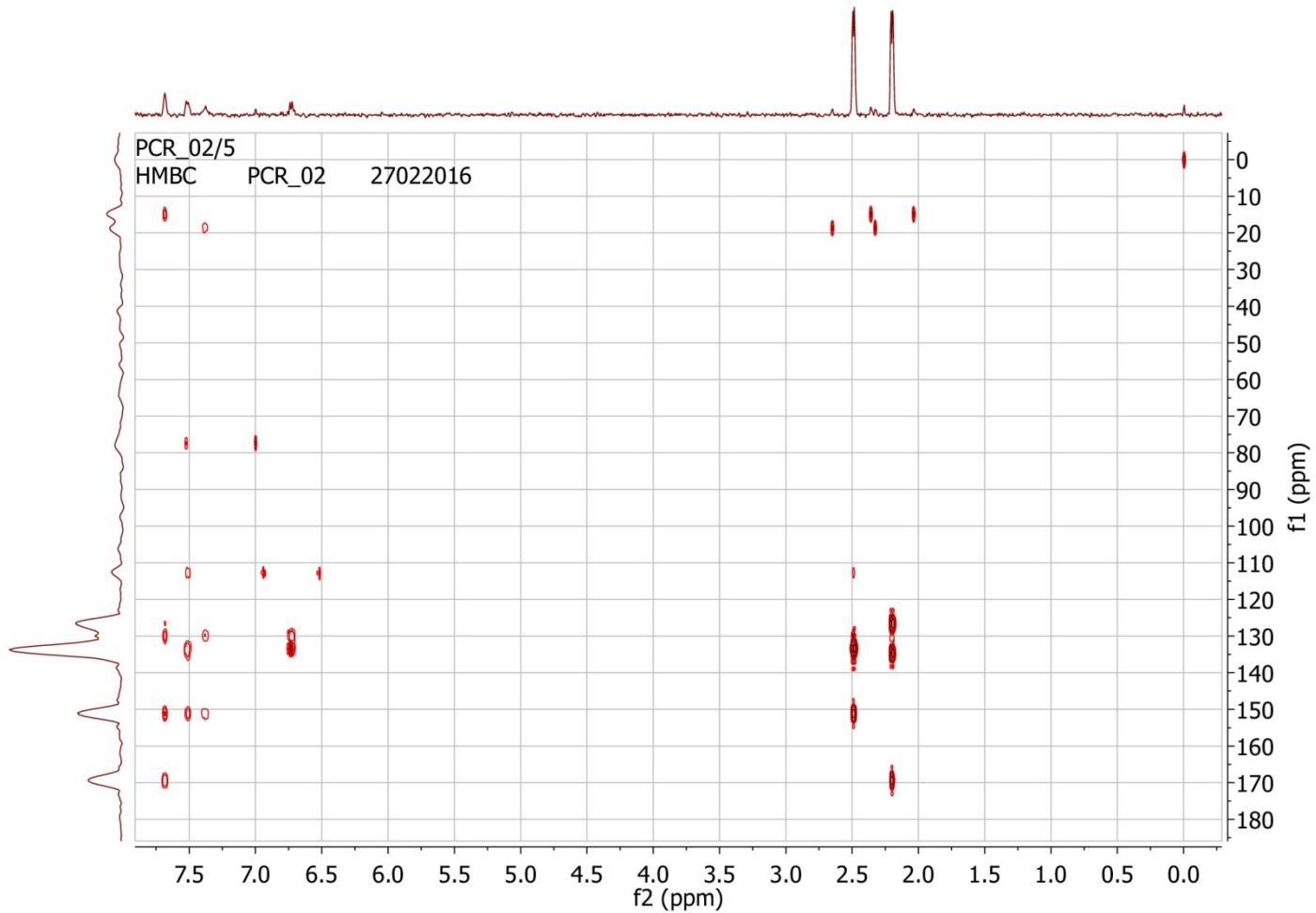
¹H NMR of **13**



¹³C NMR of 13

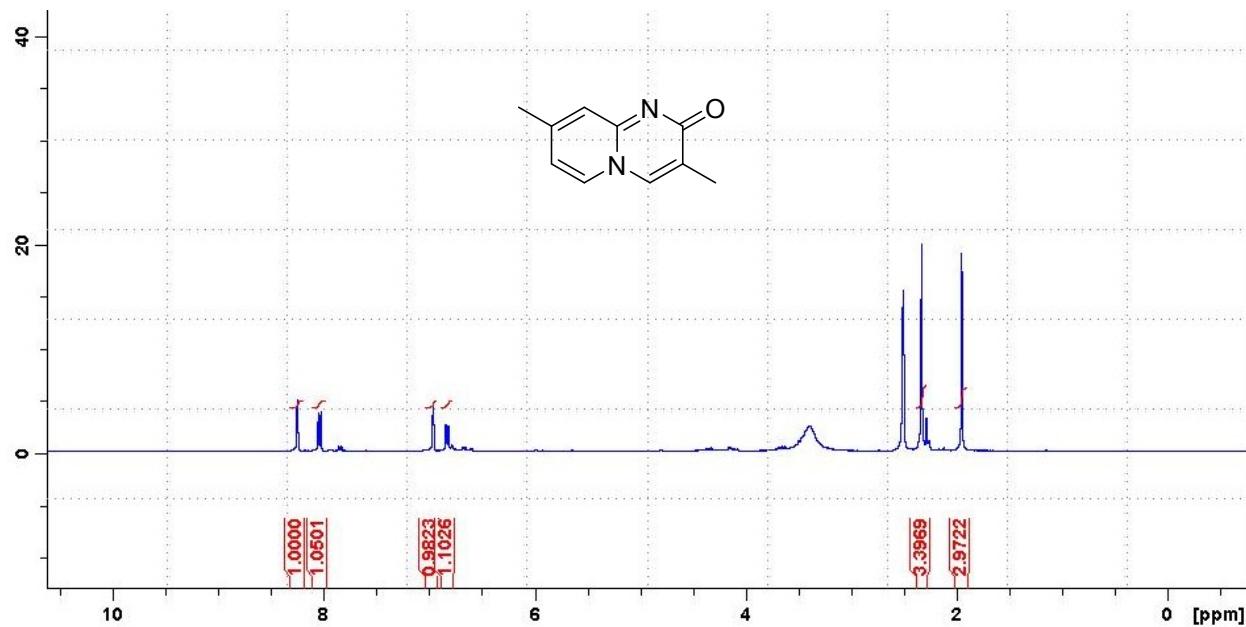


HMBC of **13** (CDCl_3)

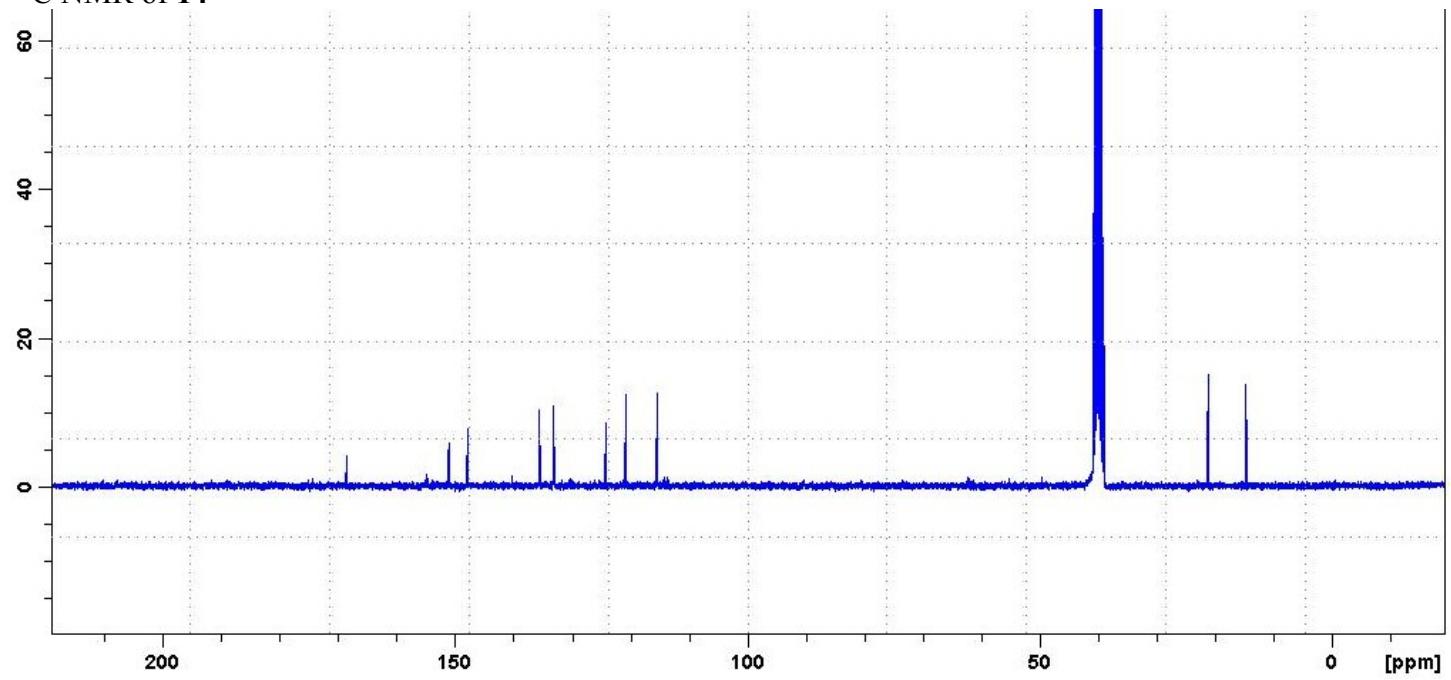


3,8-Dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (14)

¹H NMR of 14

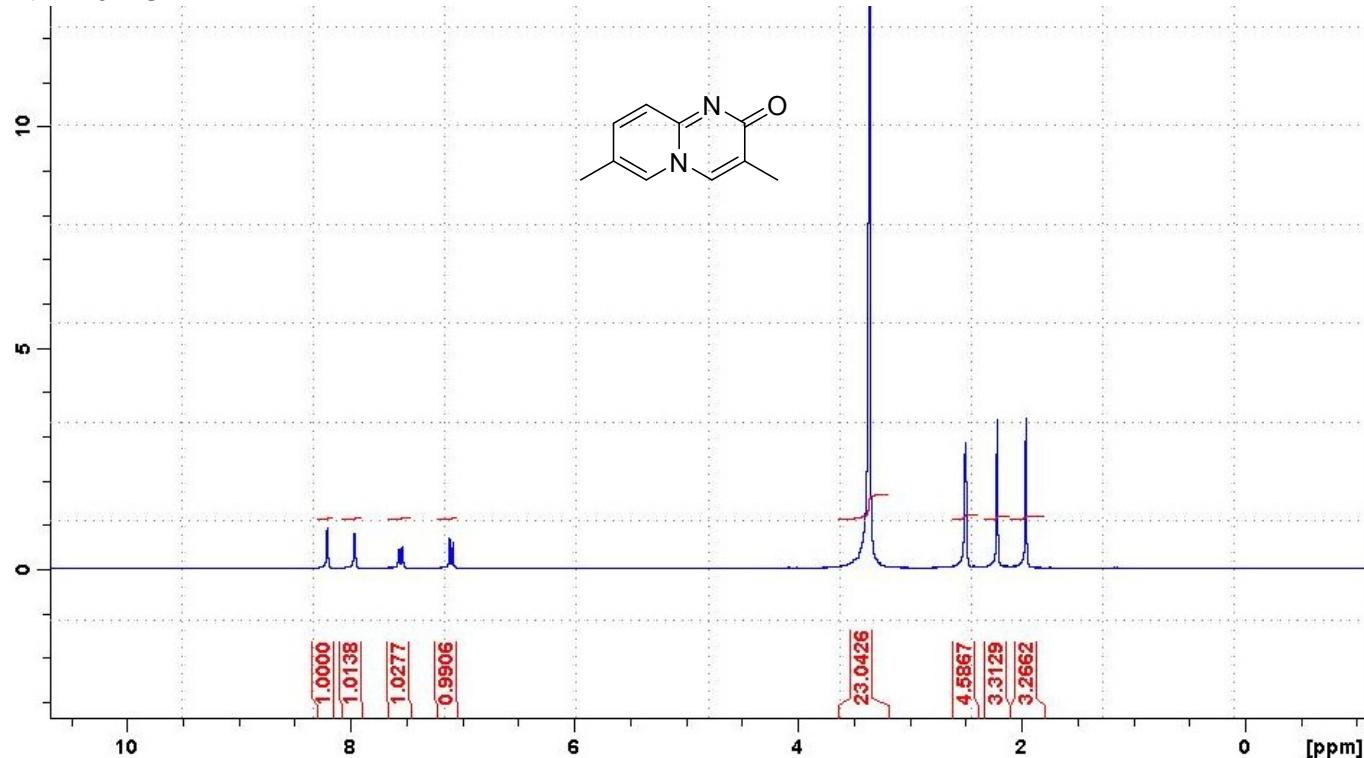


¹³C NMR of 14

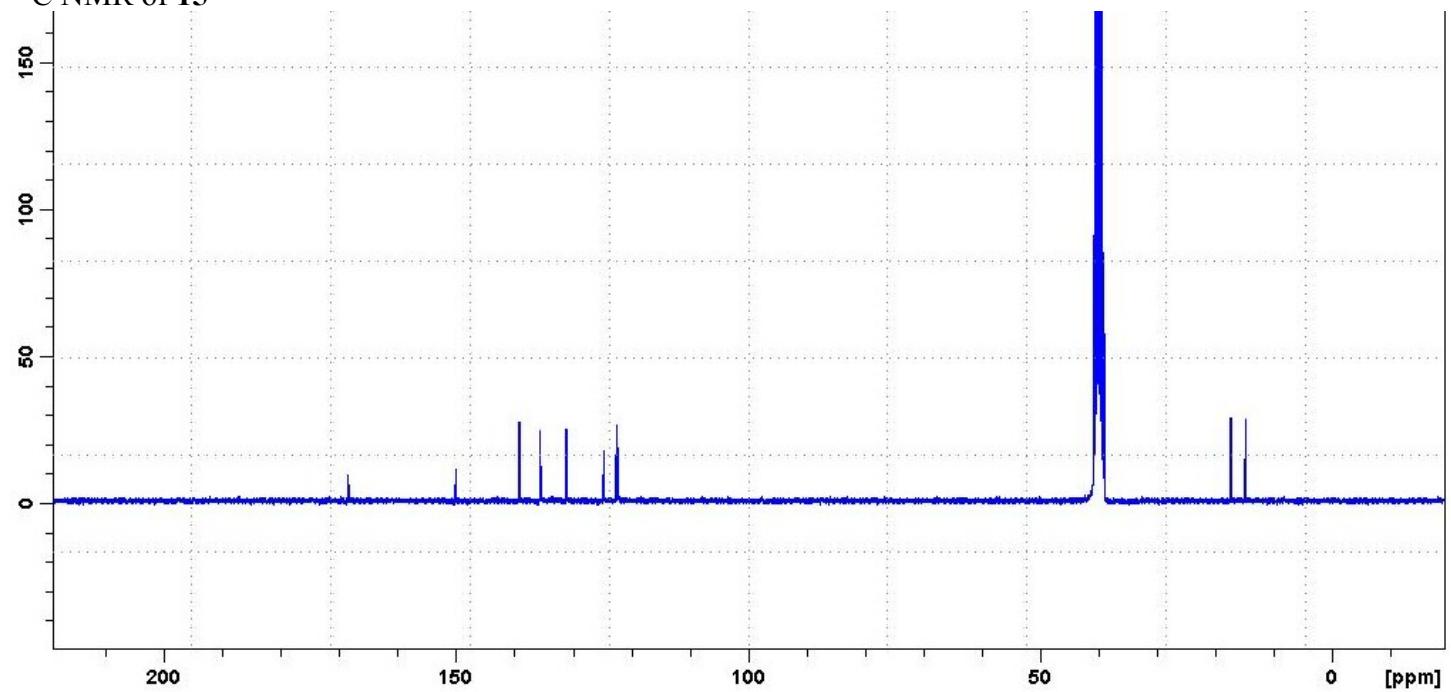


3,7-Dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (15)

¹H NMR of **15**

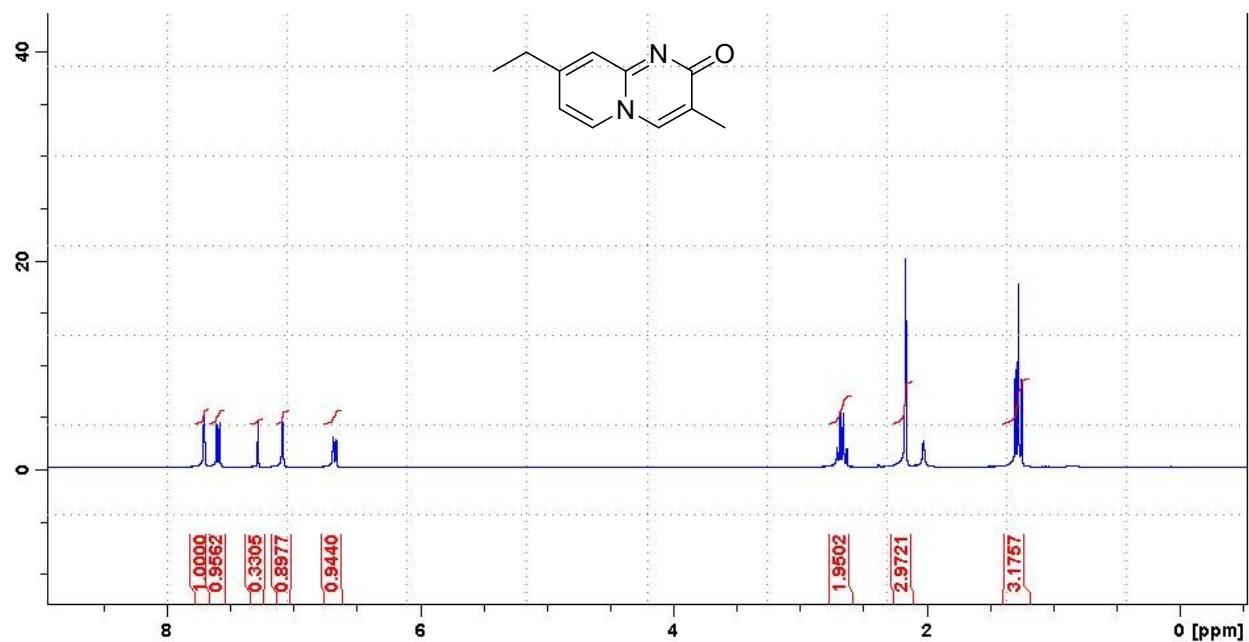


¹³C NMR of **15**

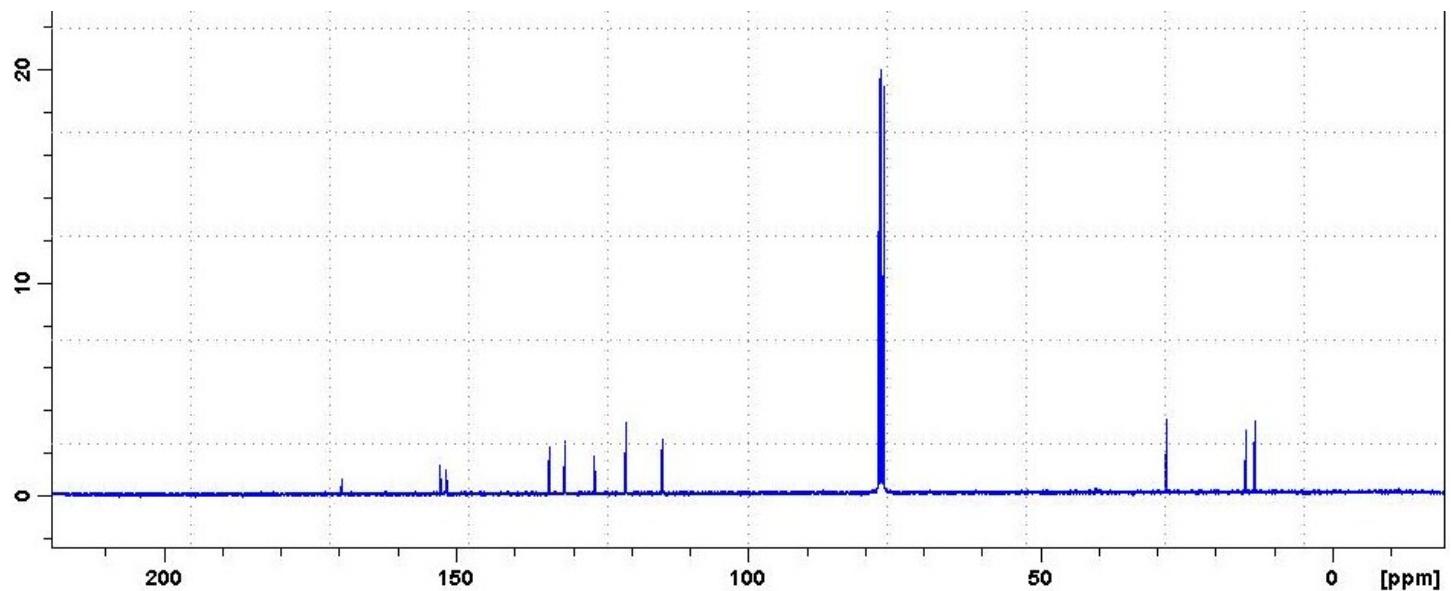


8-Ethyl-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (16)

¹H NMR of **16**

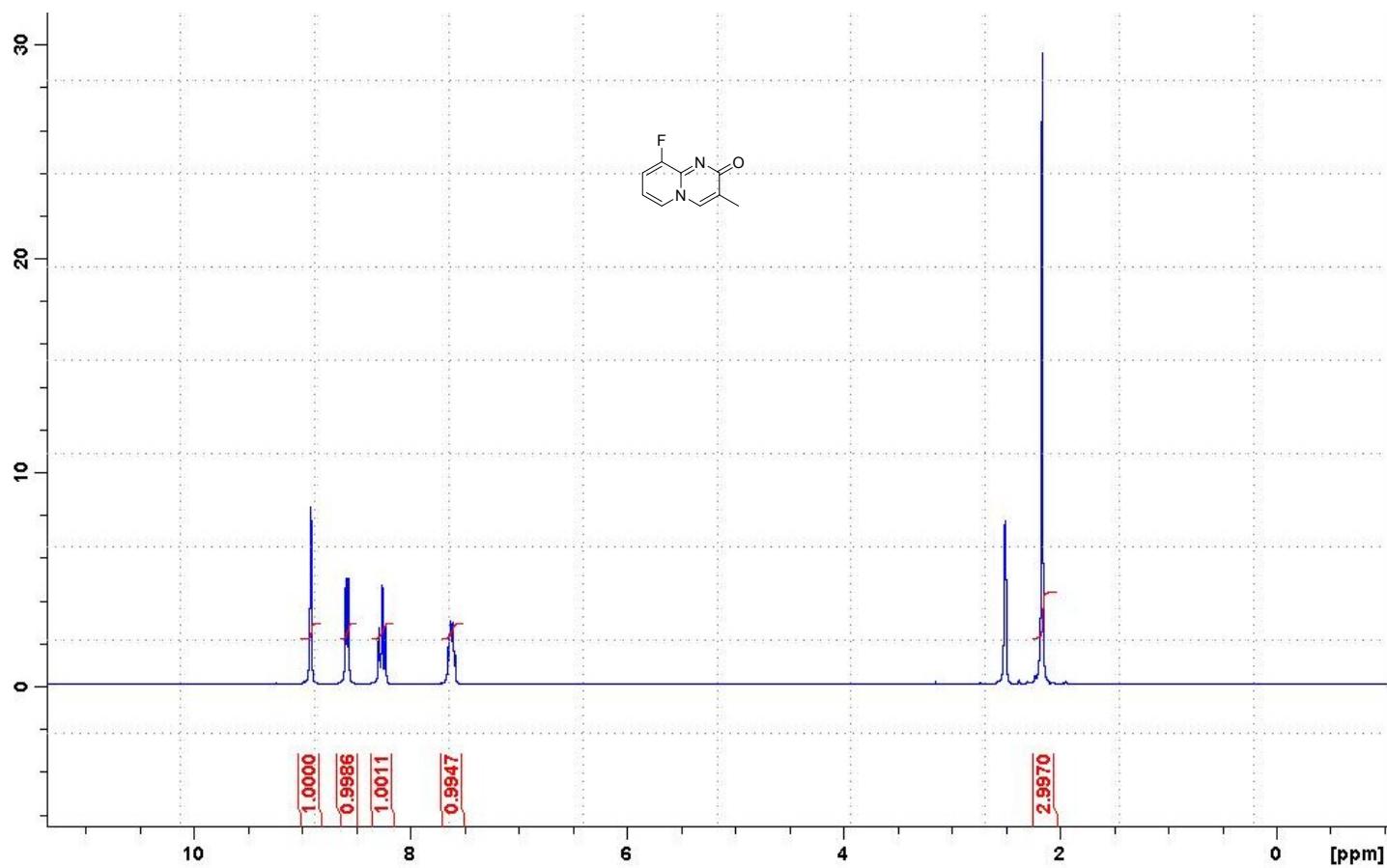


¹³C NMR of **16**

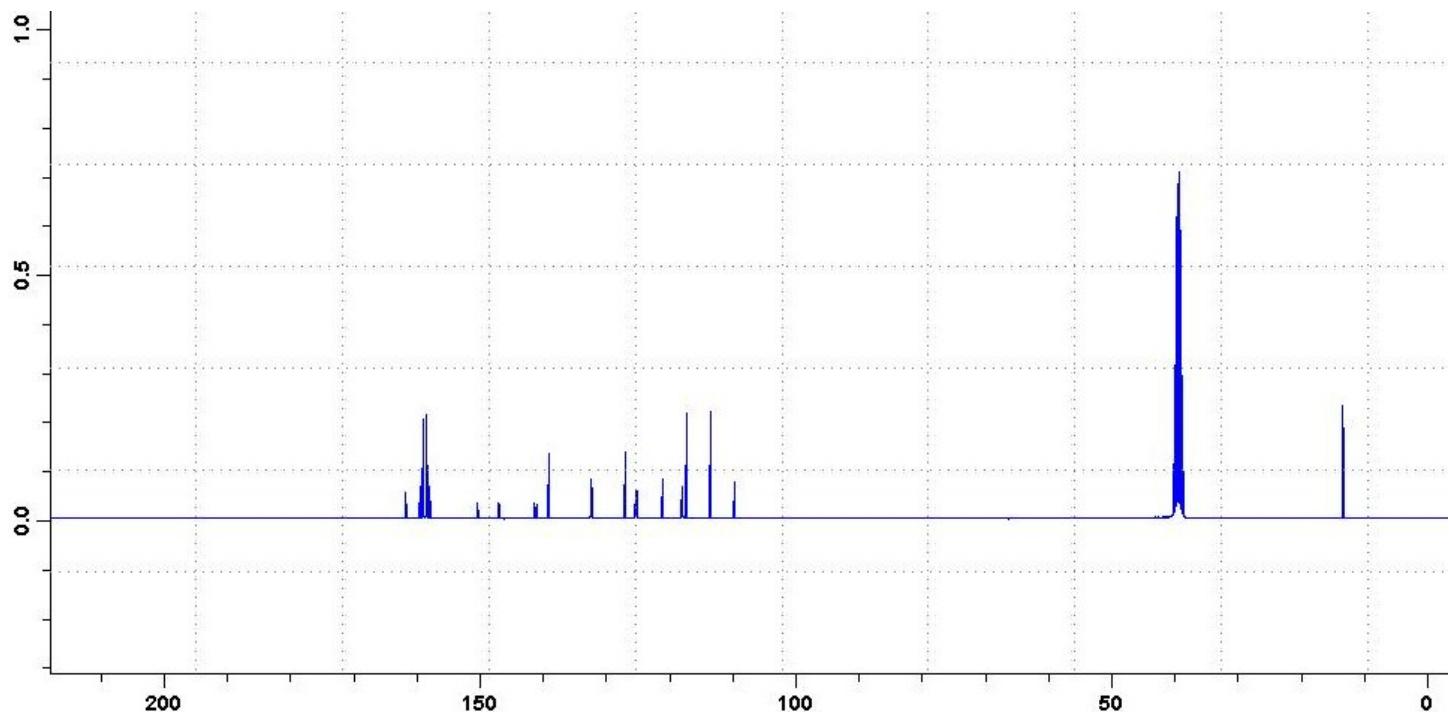


9-Fluoro-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (17)

¹H NMR of 17

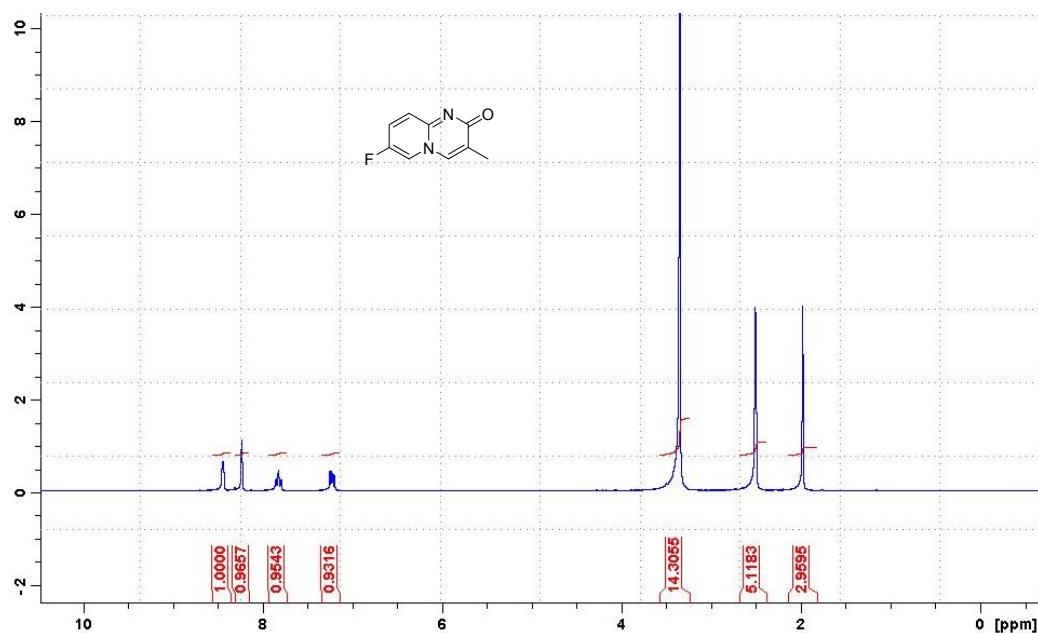


¹³C NMR of 17

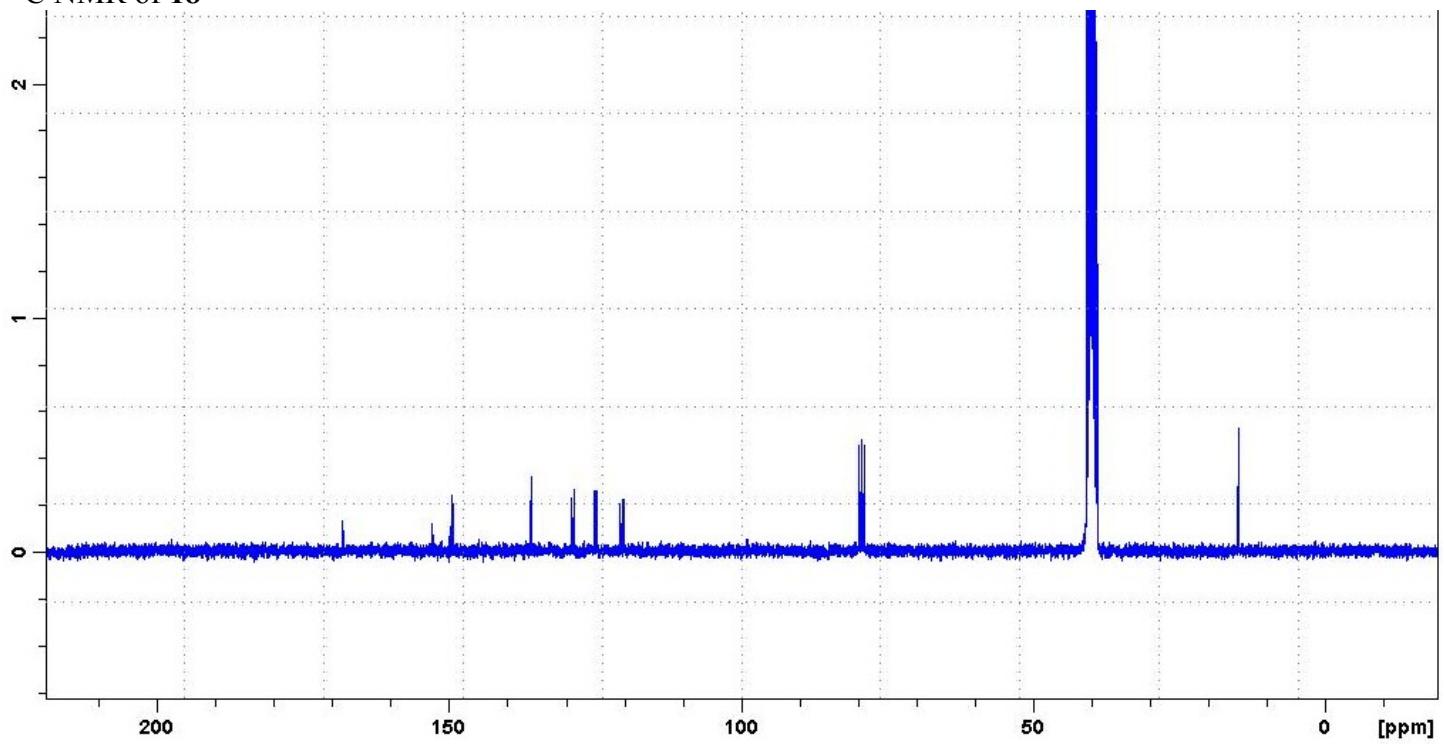


7-Fluoro-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (18)

¹H NMR of **18**

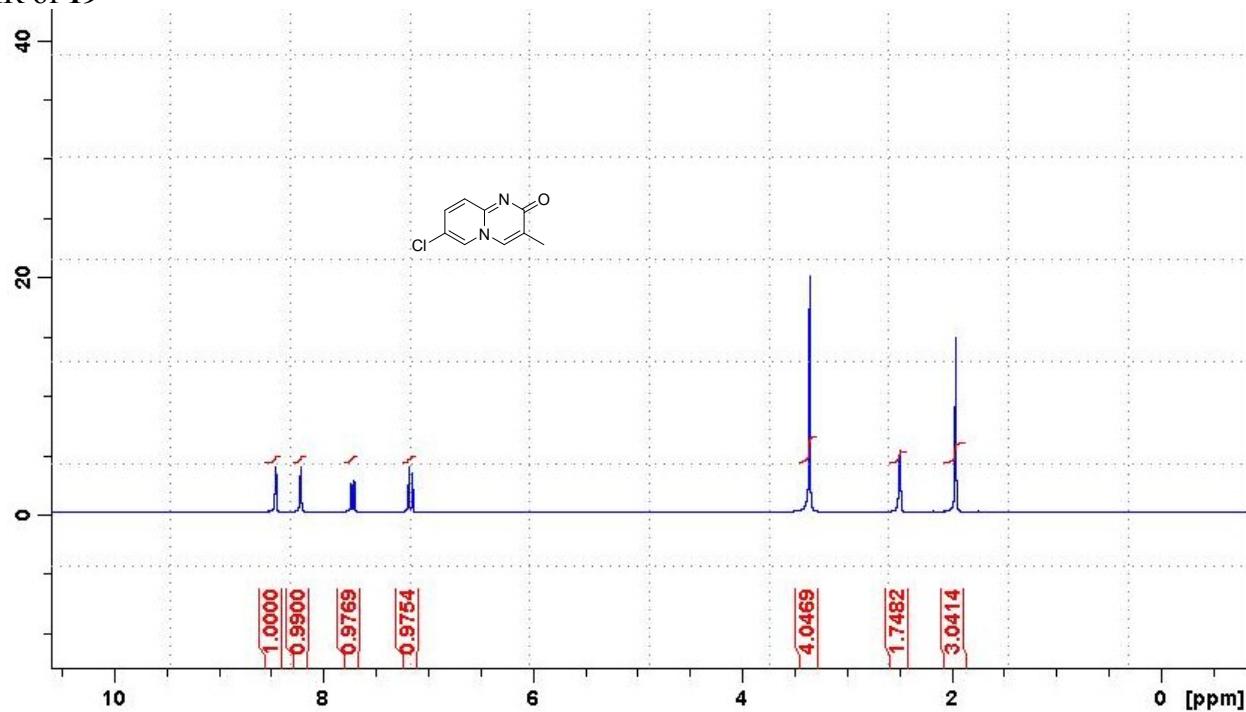


¹³C NMR of **18**

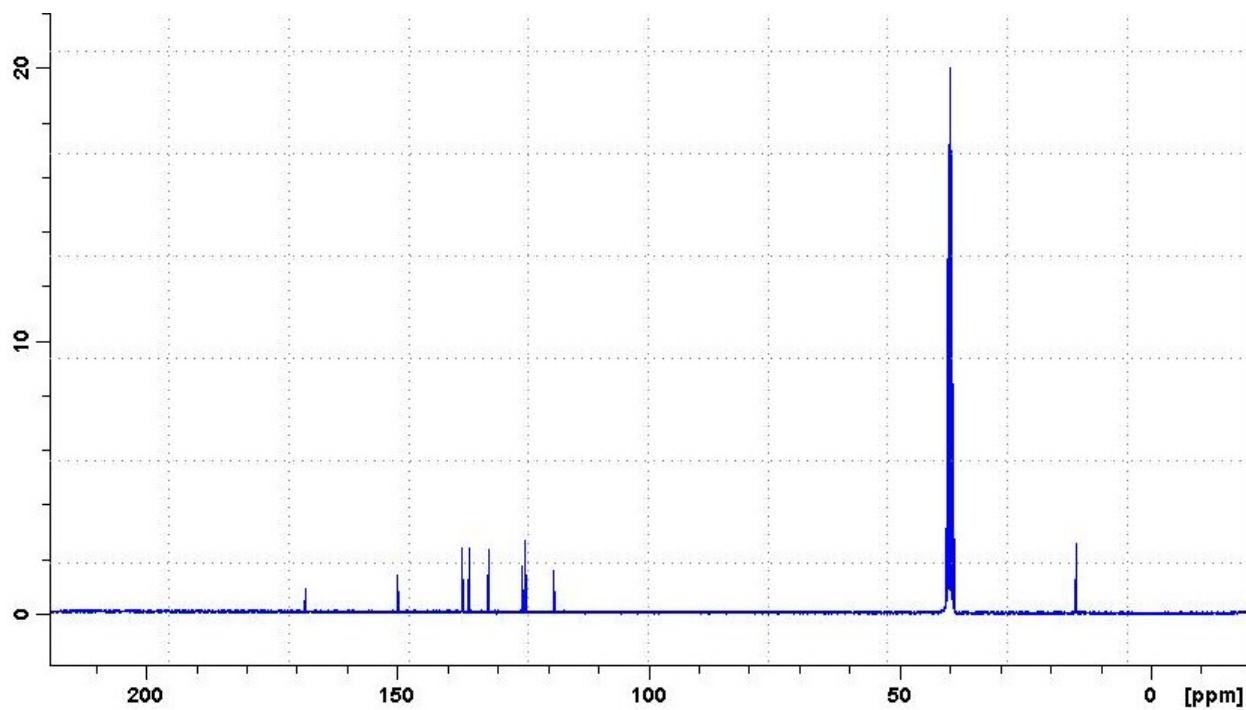


7-Chloro-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (19)

¹H NMR of **19**

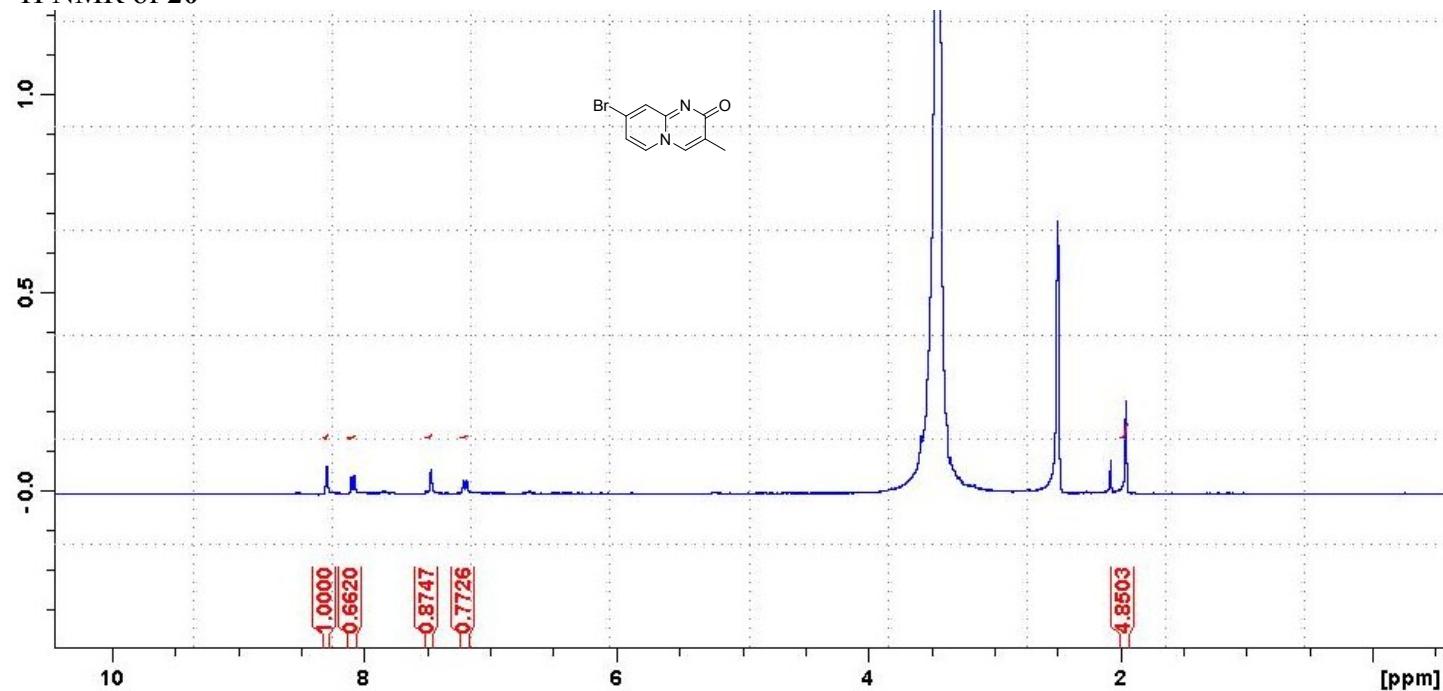


¹³C NMR of **19**

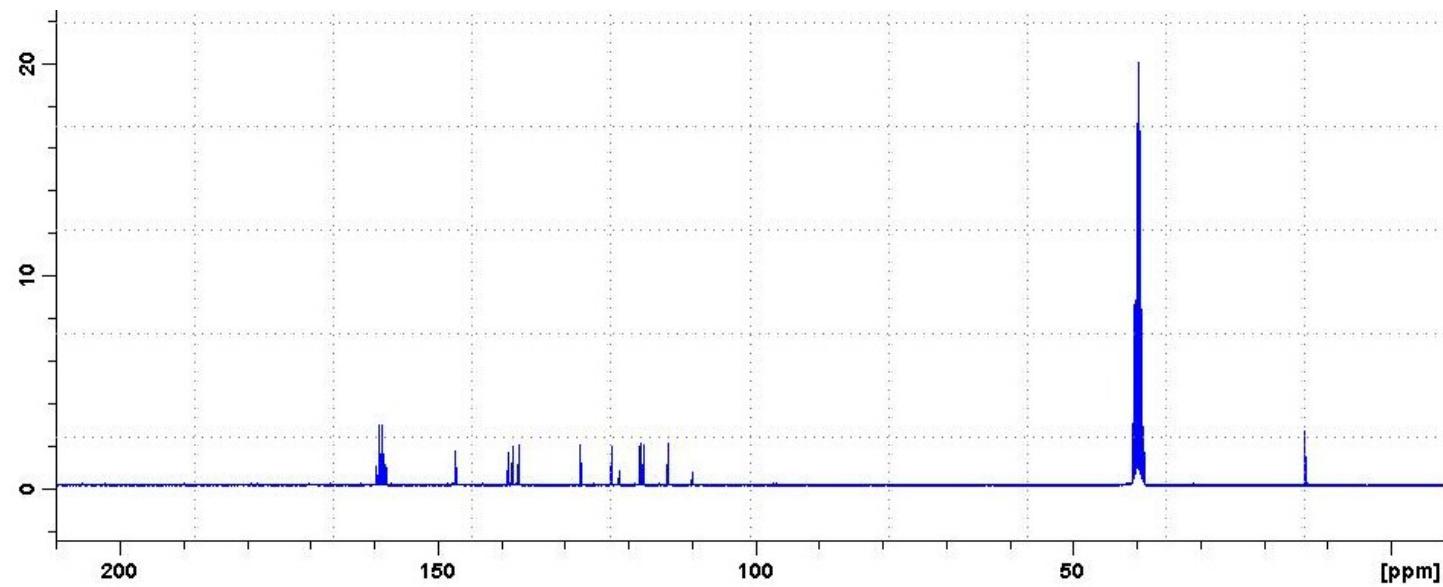


8-Bromo-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (20)

¹H NMR of **20**

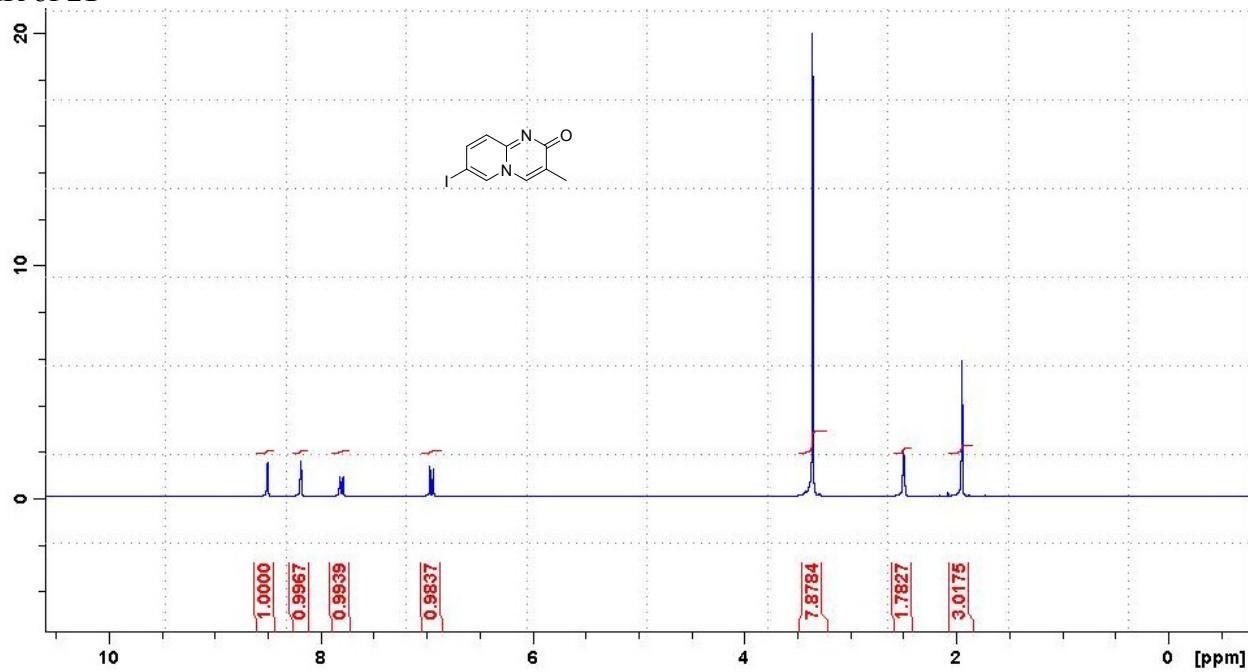


¹³C NMR of **20**

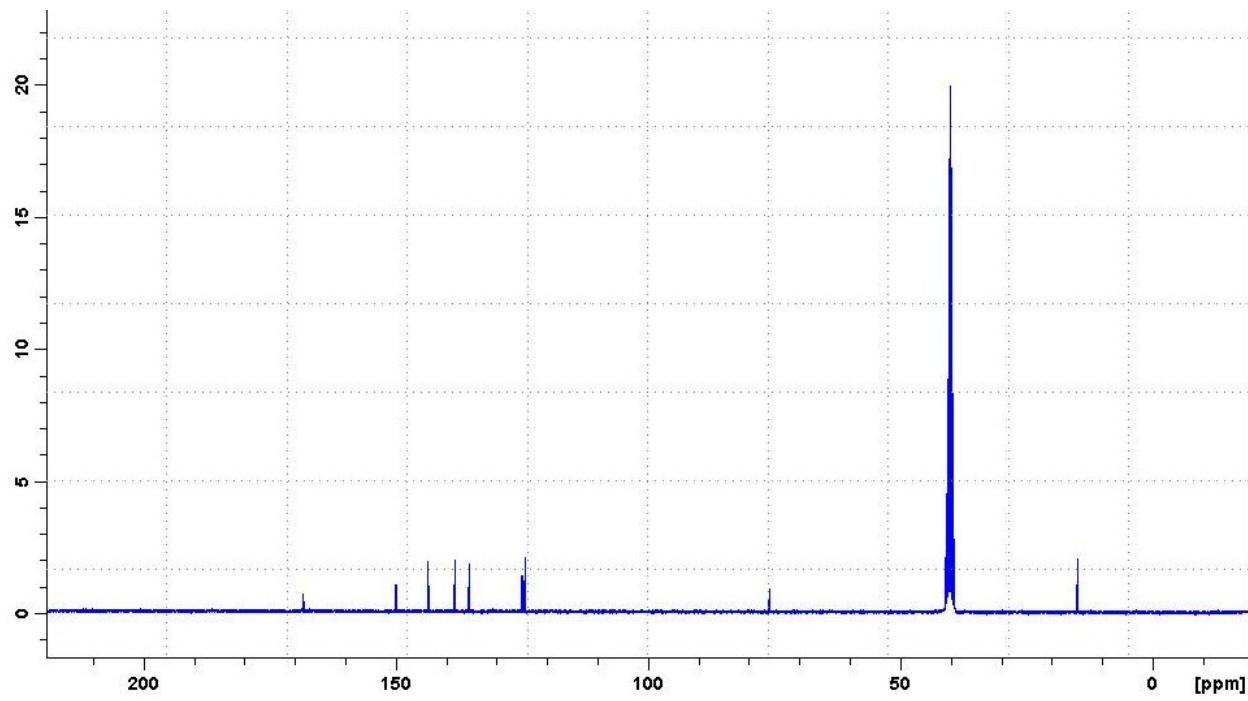


7-Iodo-3-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (21**)**

¹H NMR of **21**

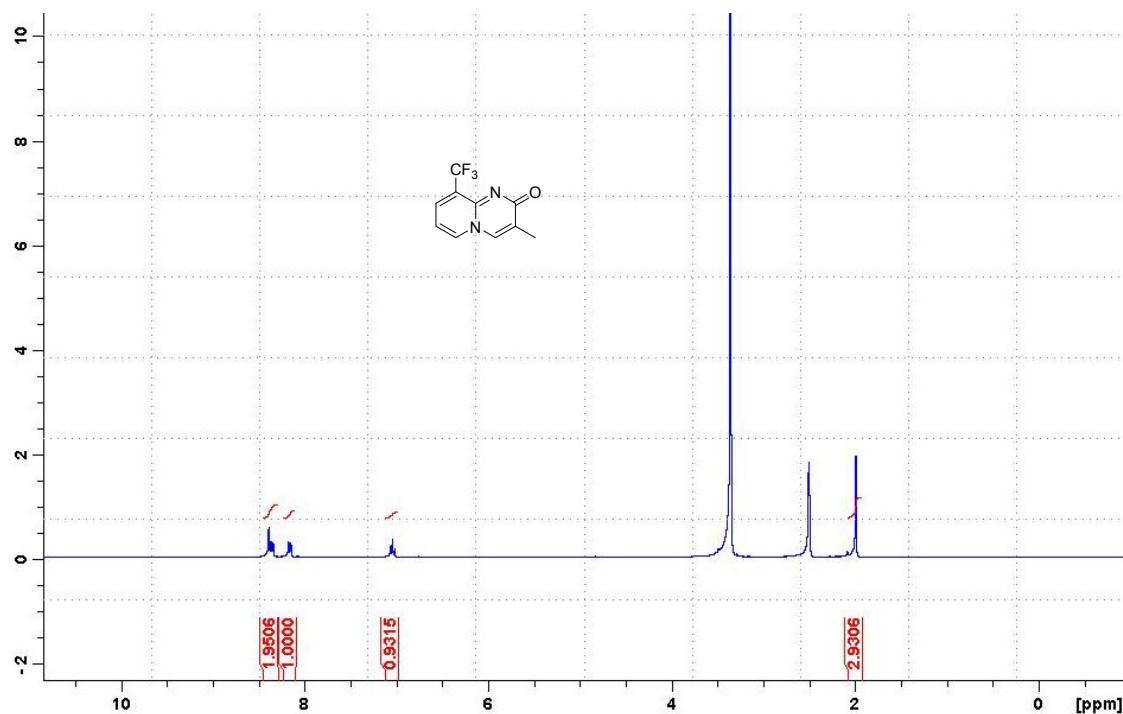


¹³C NMR of **21**

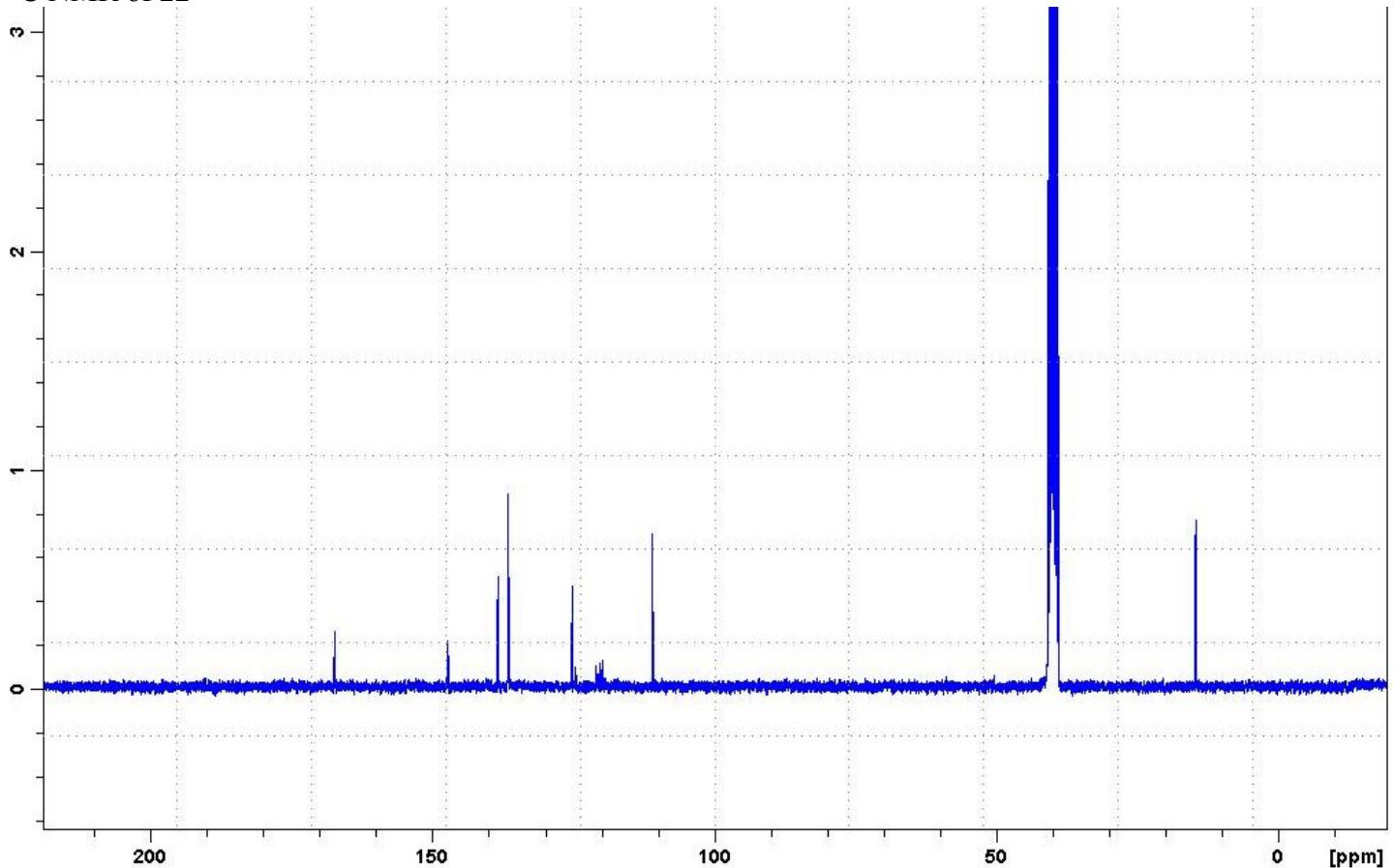


3-Methyl-9-(trifluoromethyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (22)

¹H NMR of 22

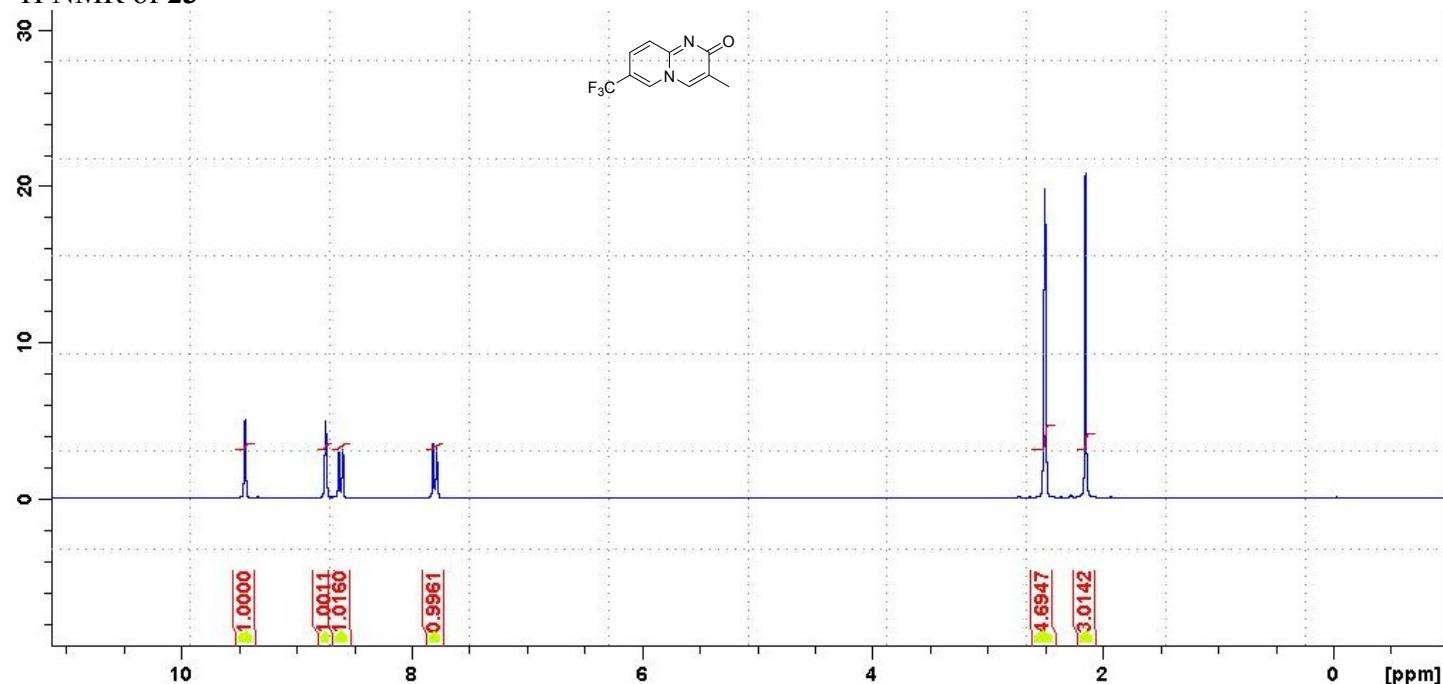


¹³C NMR of 22

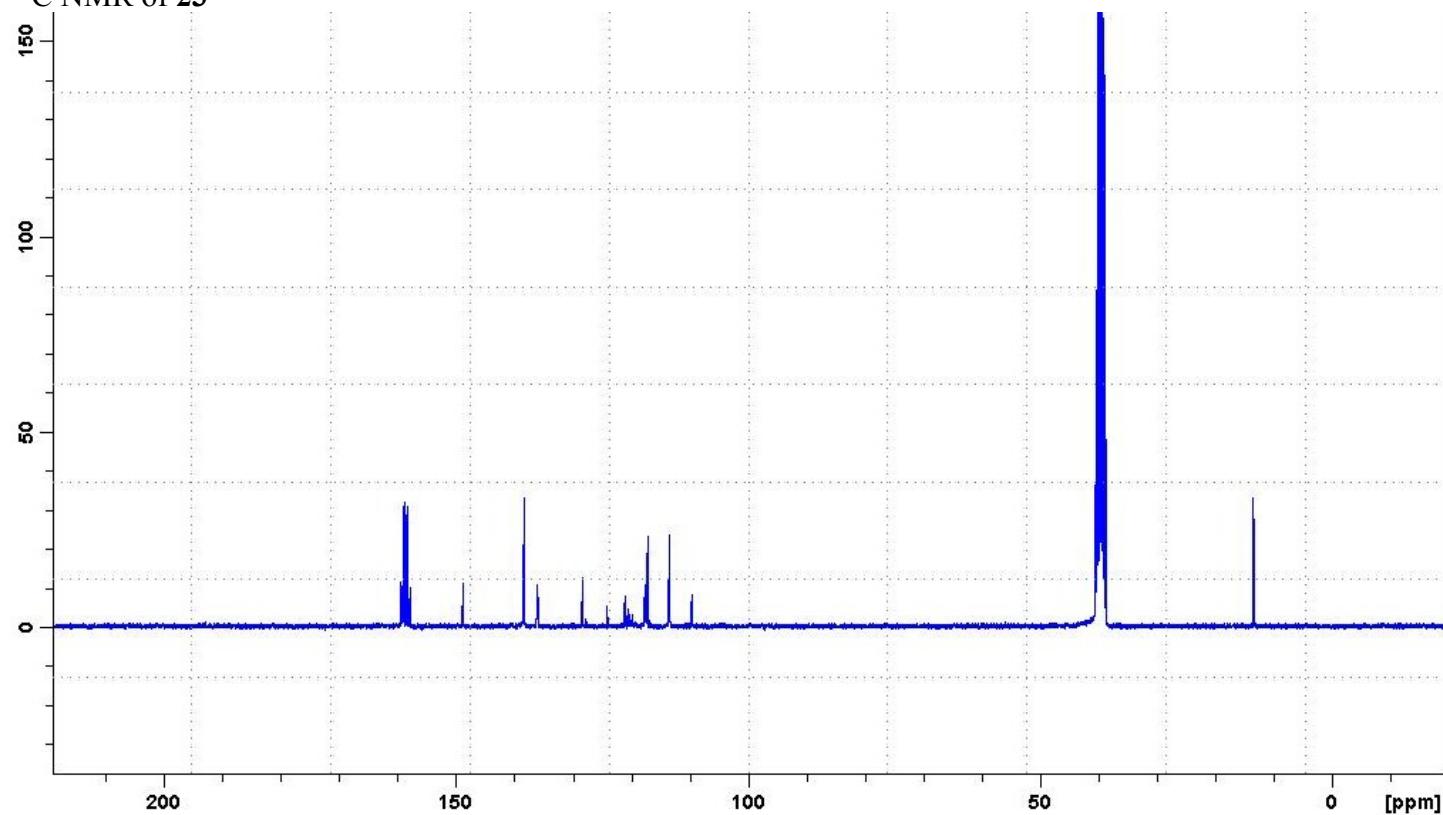


3-Methyl-7-(trifluoromethyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (23)

¹H NMR of 23

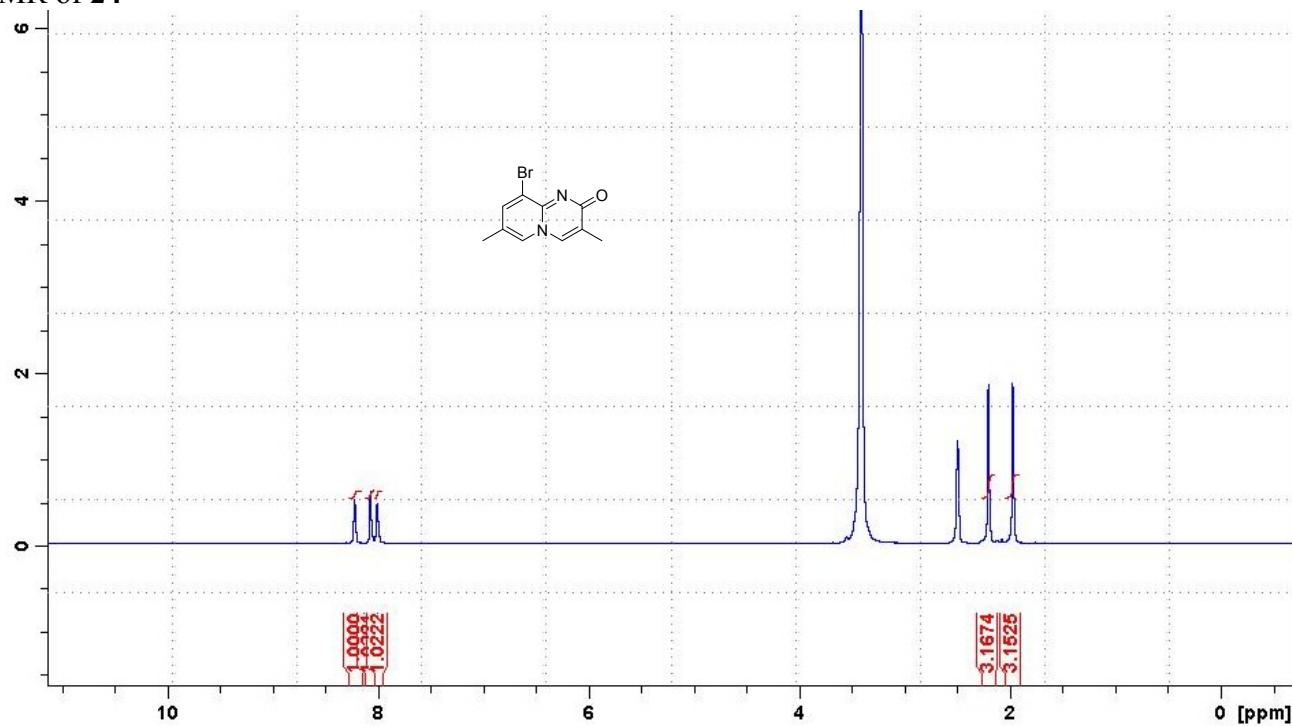


¹³C NMR of 23

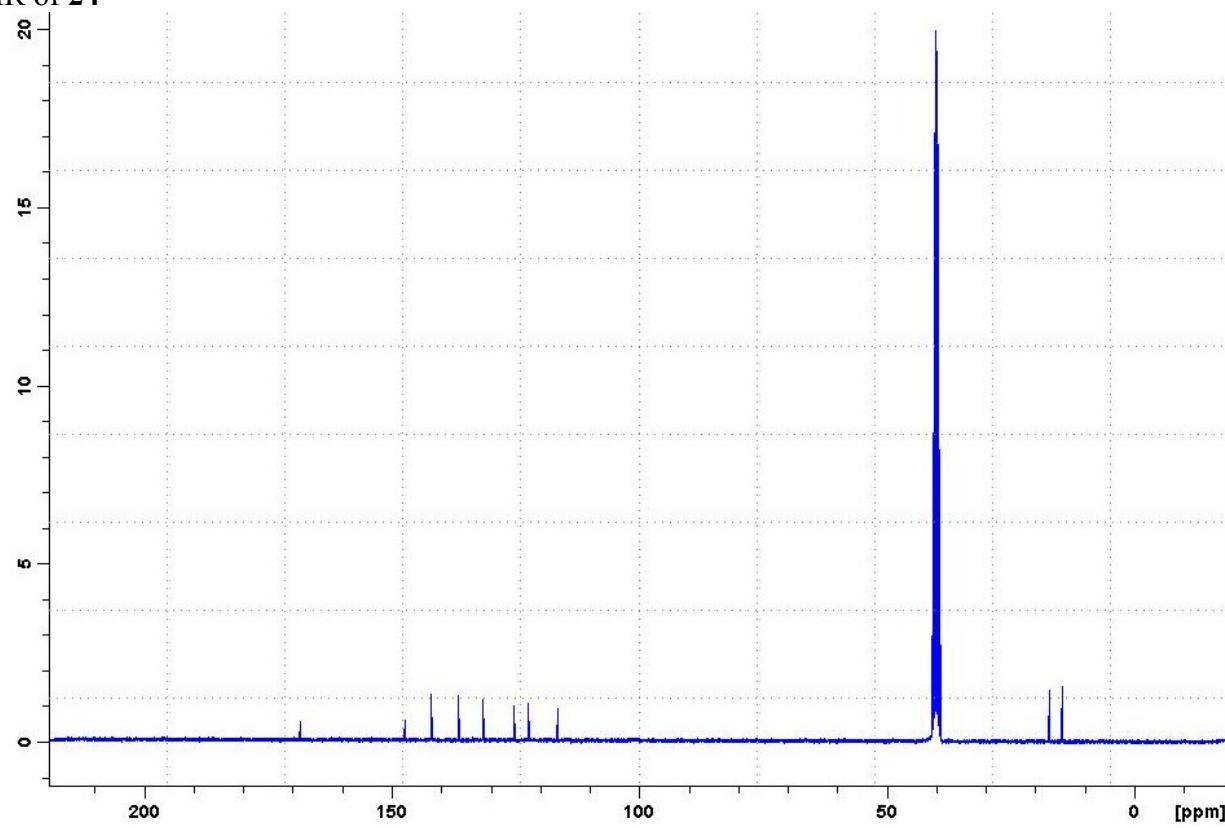


9-Bromo-3,7-dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (24)

¹H NMR of 24

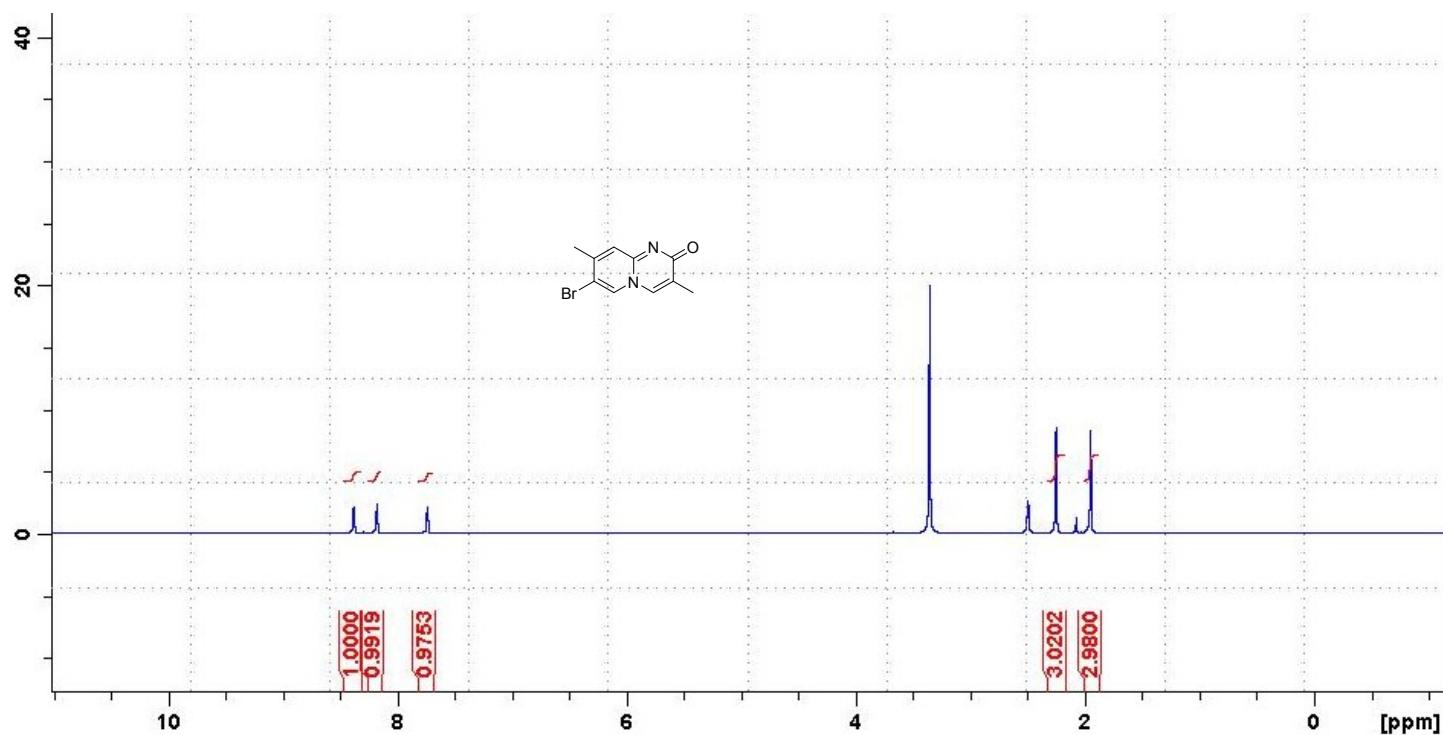


¹³C NMR of 24

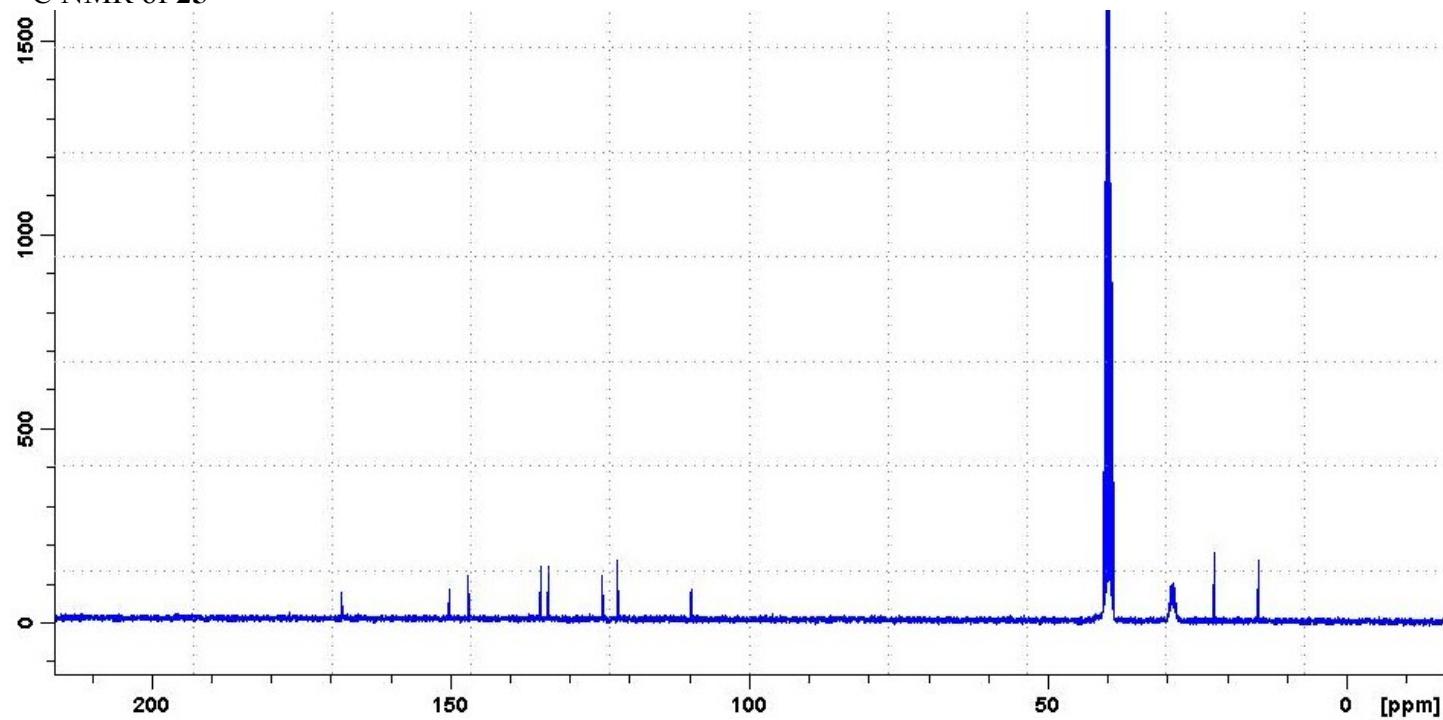


7-Bromo-3,8-dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (25)

¹H NMR of 25

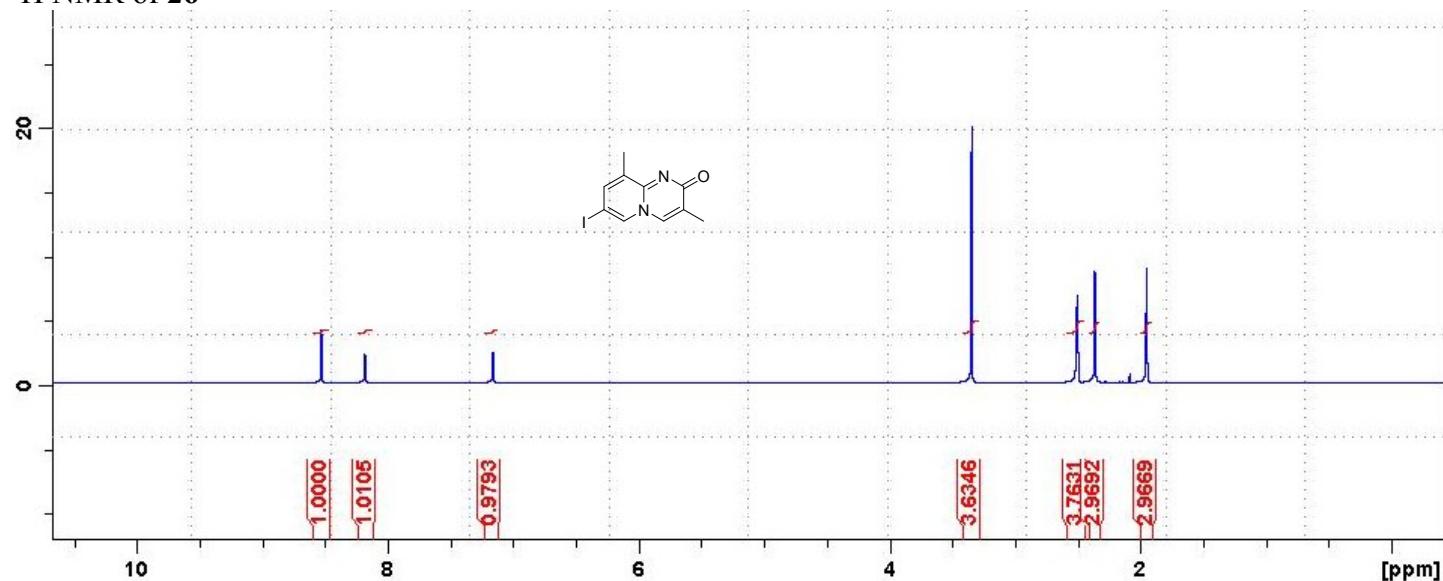


¹³C NMR of 25

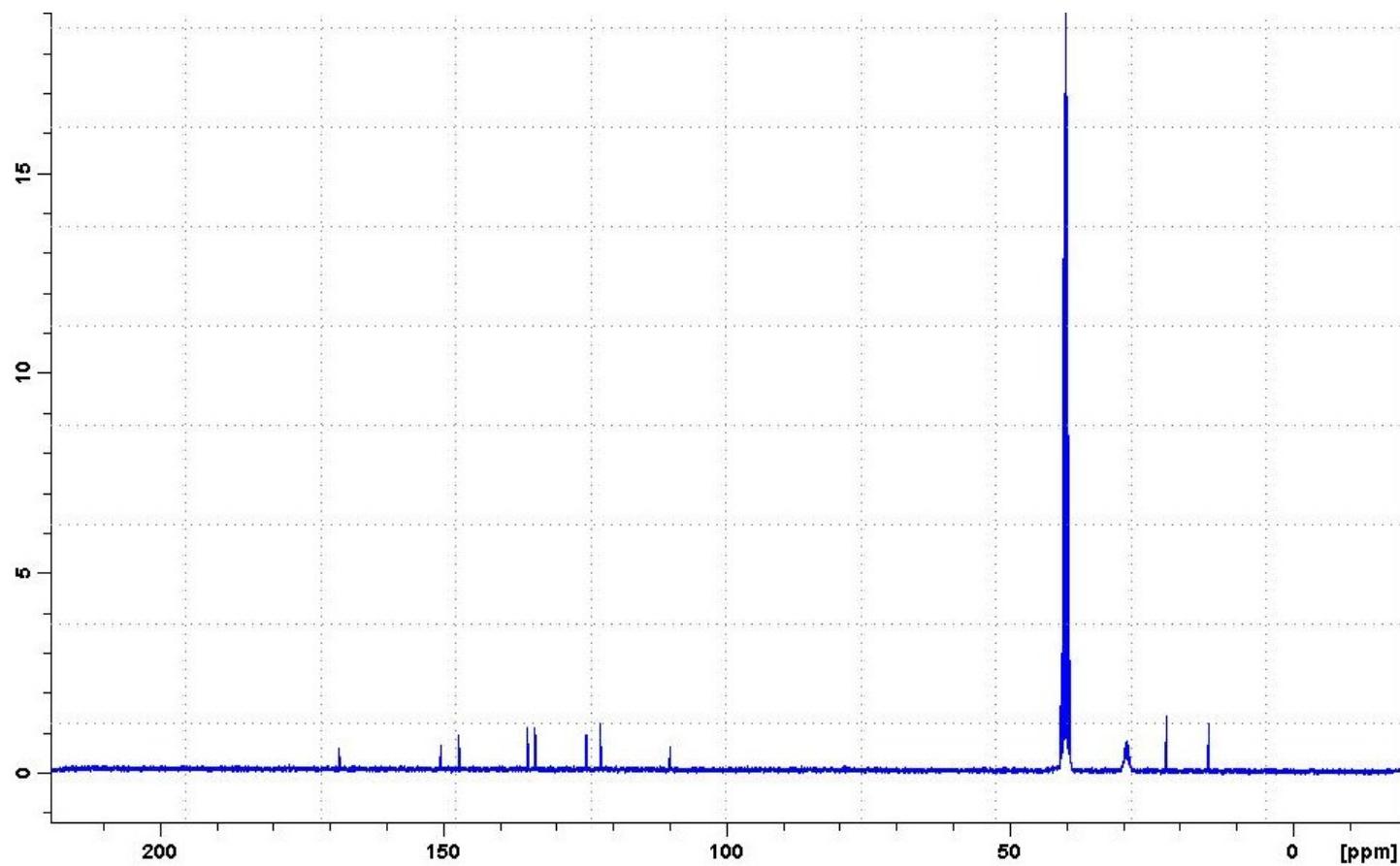


7-Iodo-3,9-dimethyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (26)

¹H NMR of **26**

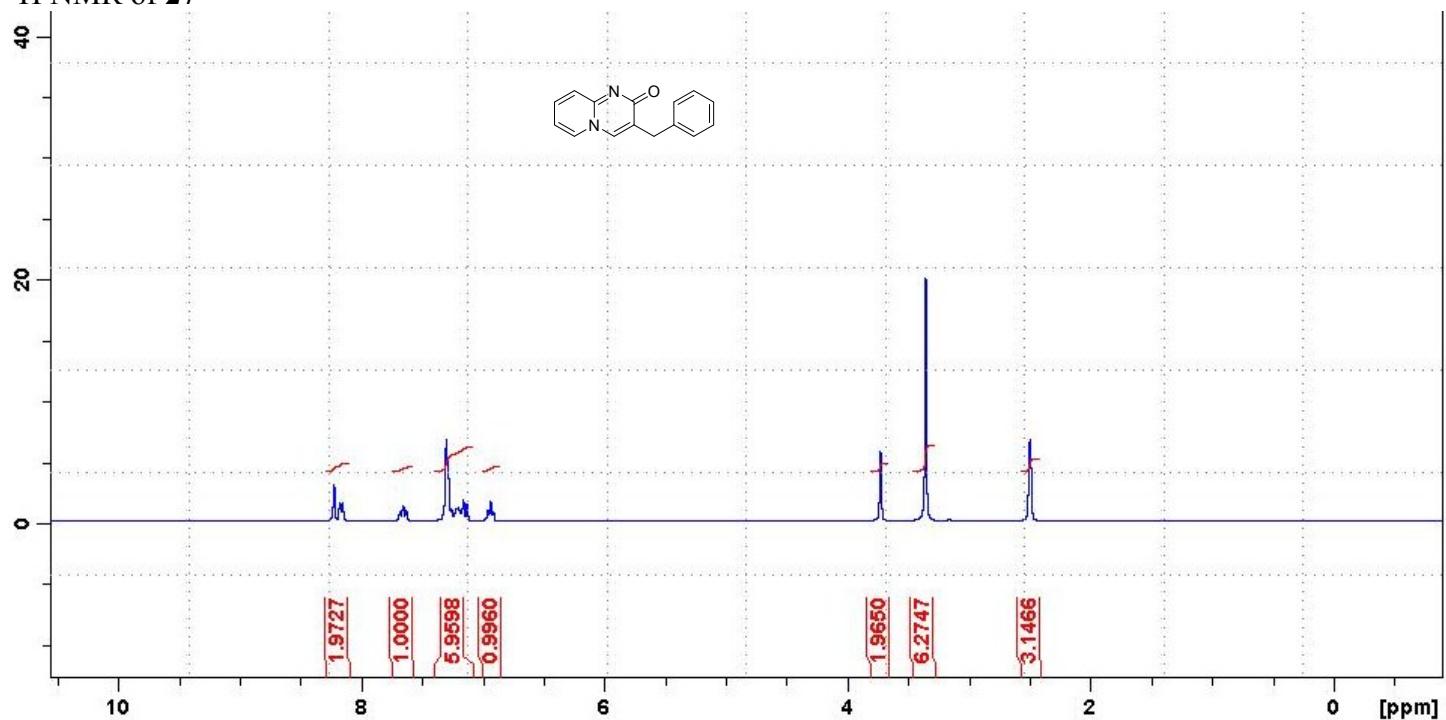


¹³C NMR of **26**

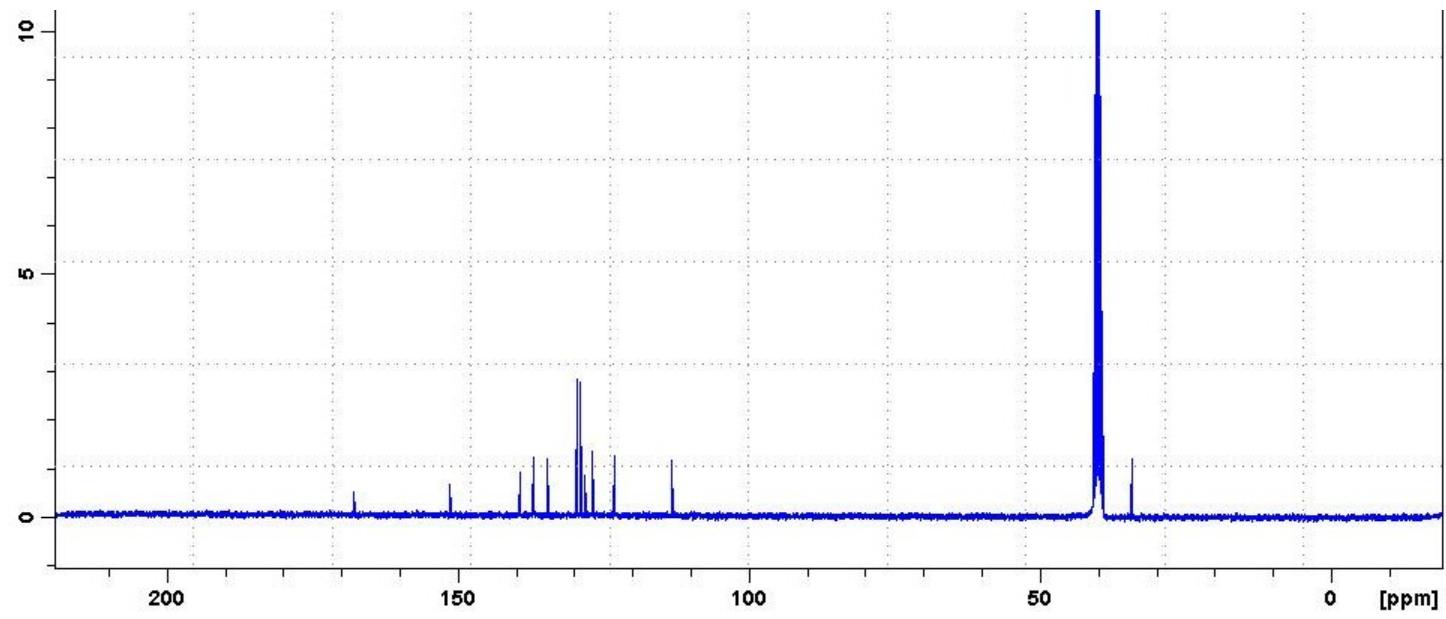


3-Benzyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (27)

¹H NMR of 27

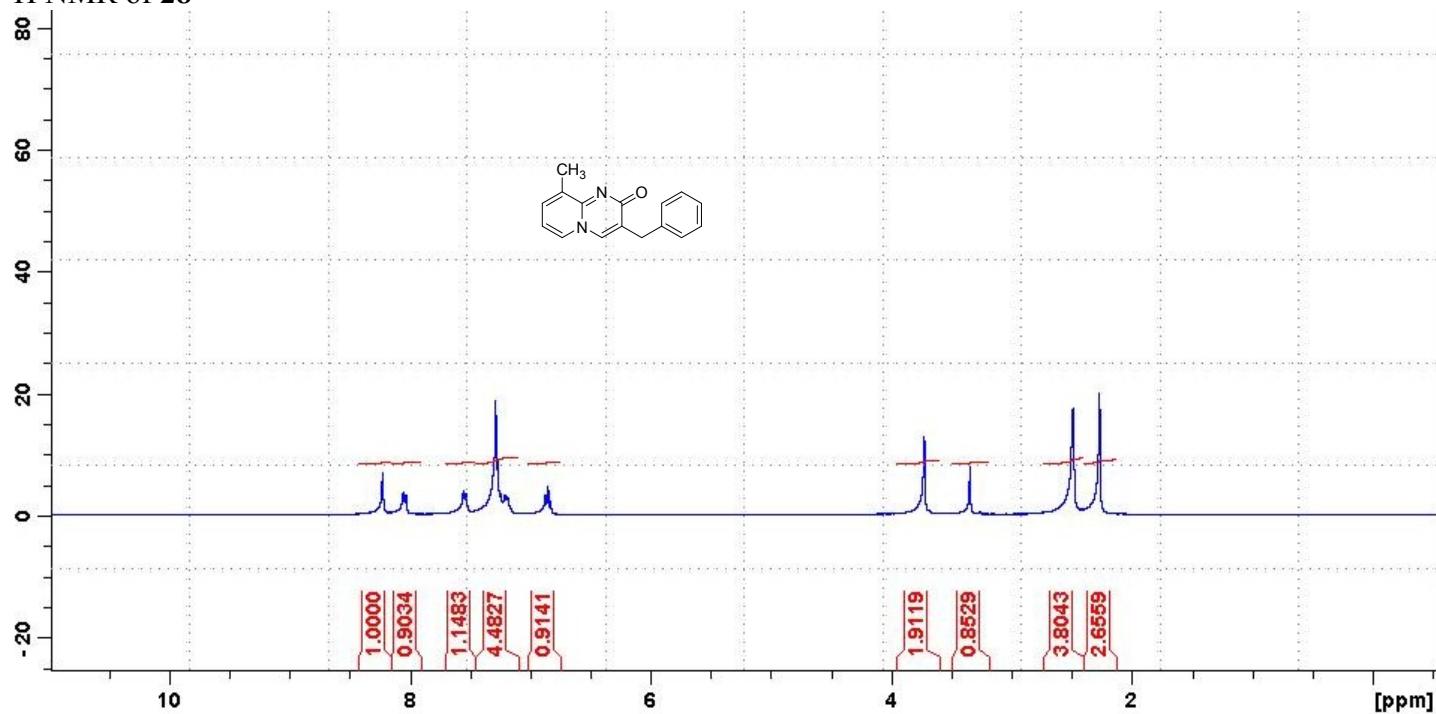


¹³C NMR of 27

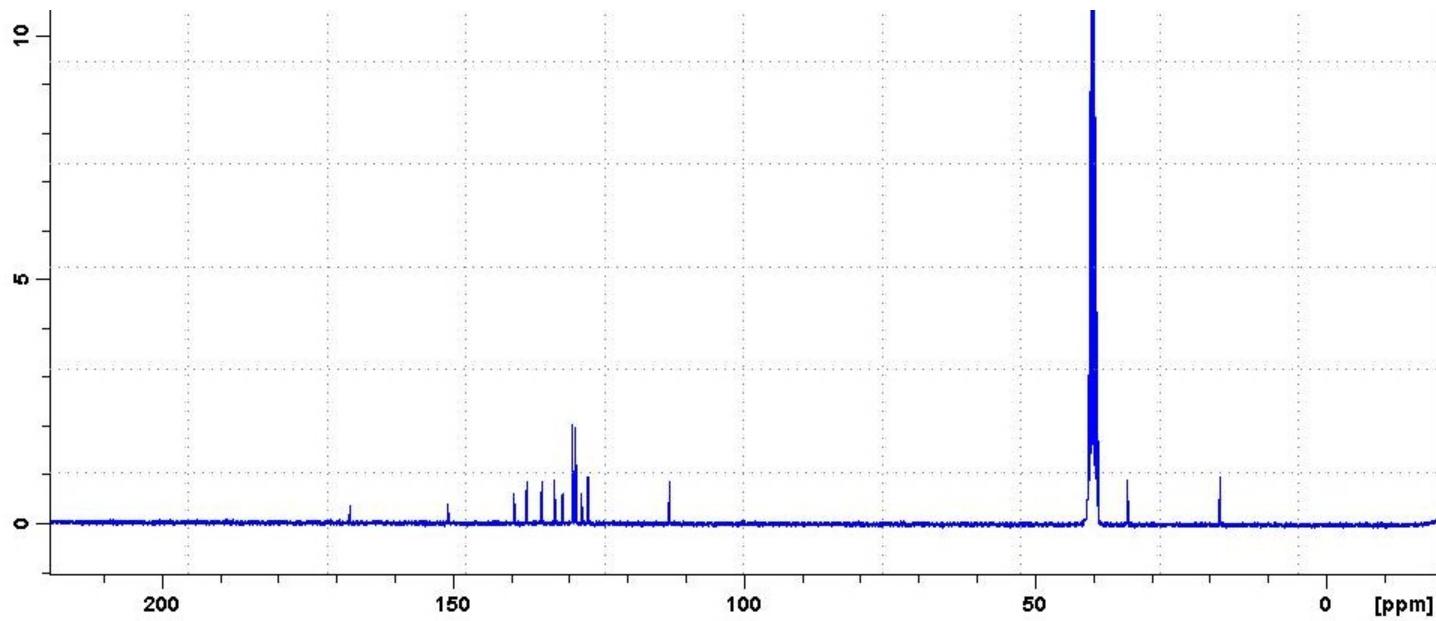


3-Benzyl-9-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (28)

¹H NMR of **28**

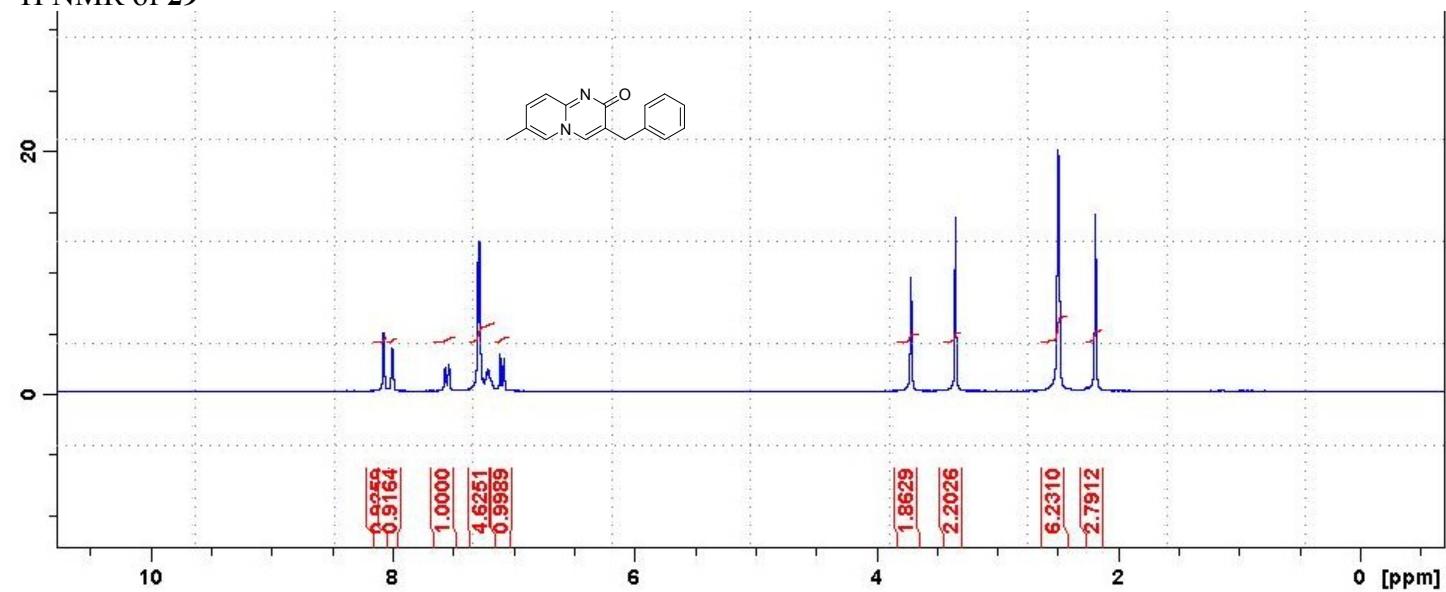


¹³C NMR of **28**

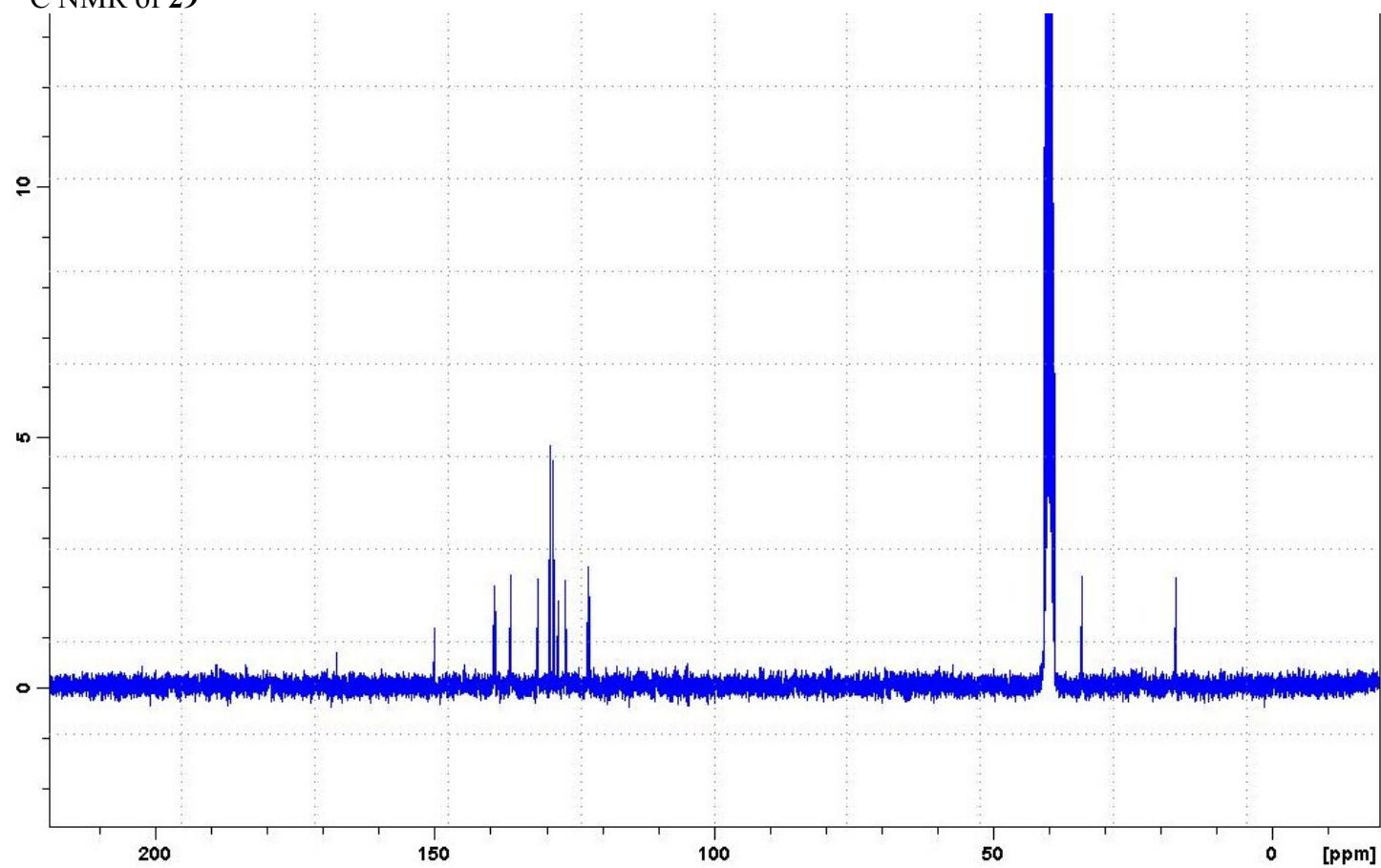


3-Benzyl-7-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (29)

¹H NMR of **29**

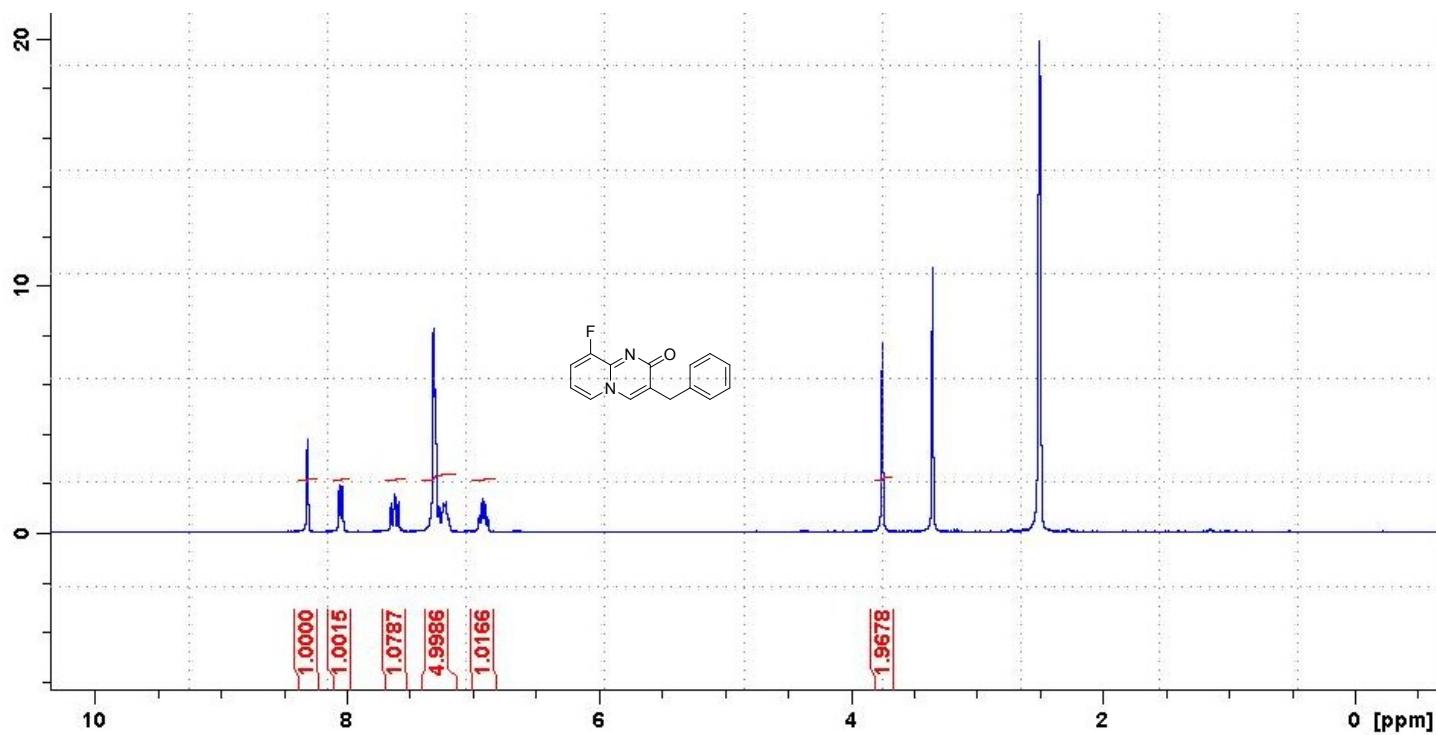


¹³C NMR of **29**

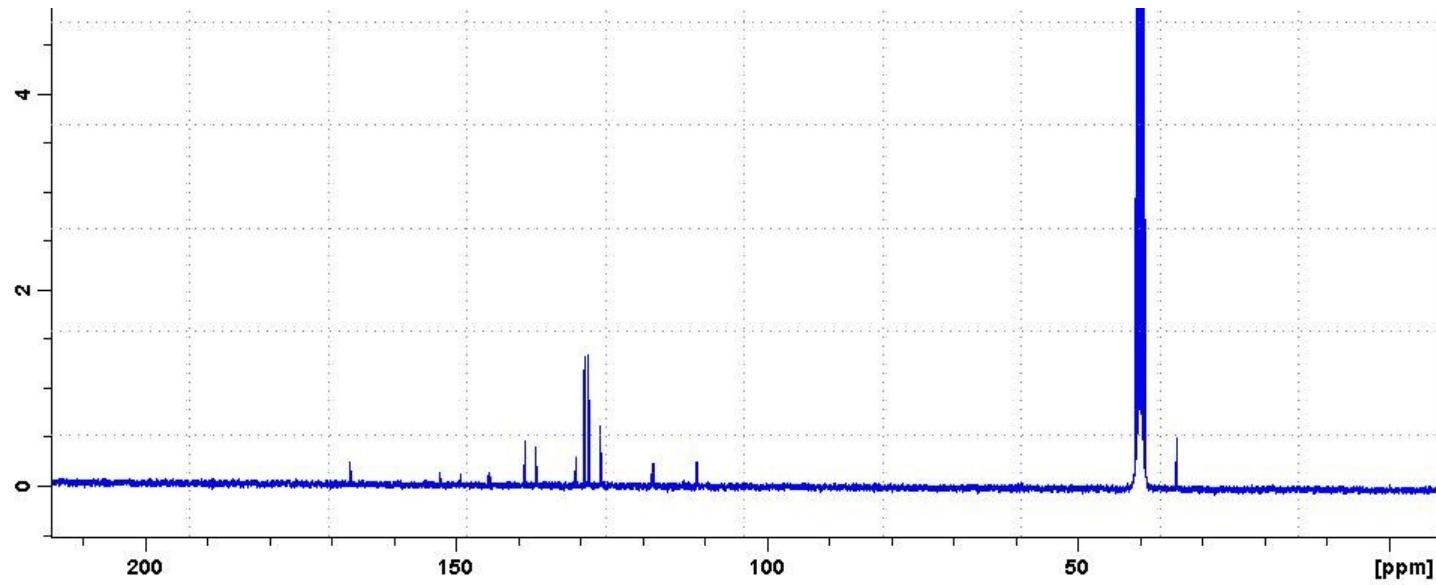


3-Benzyl-9-fluoro-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (30)

¹H NMR of **30**

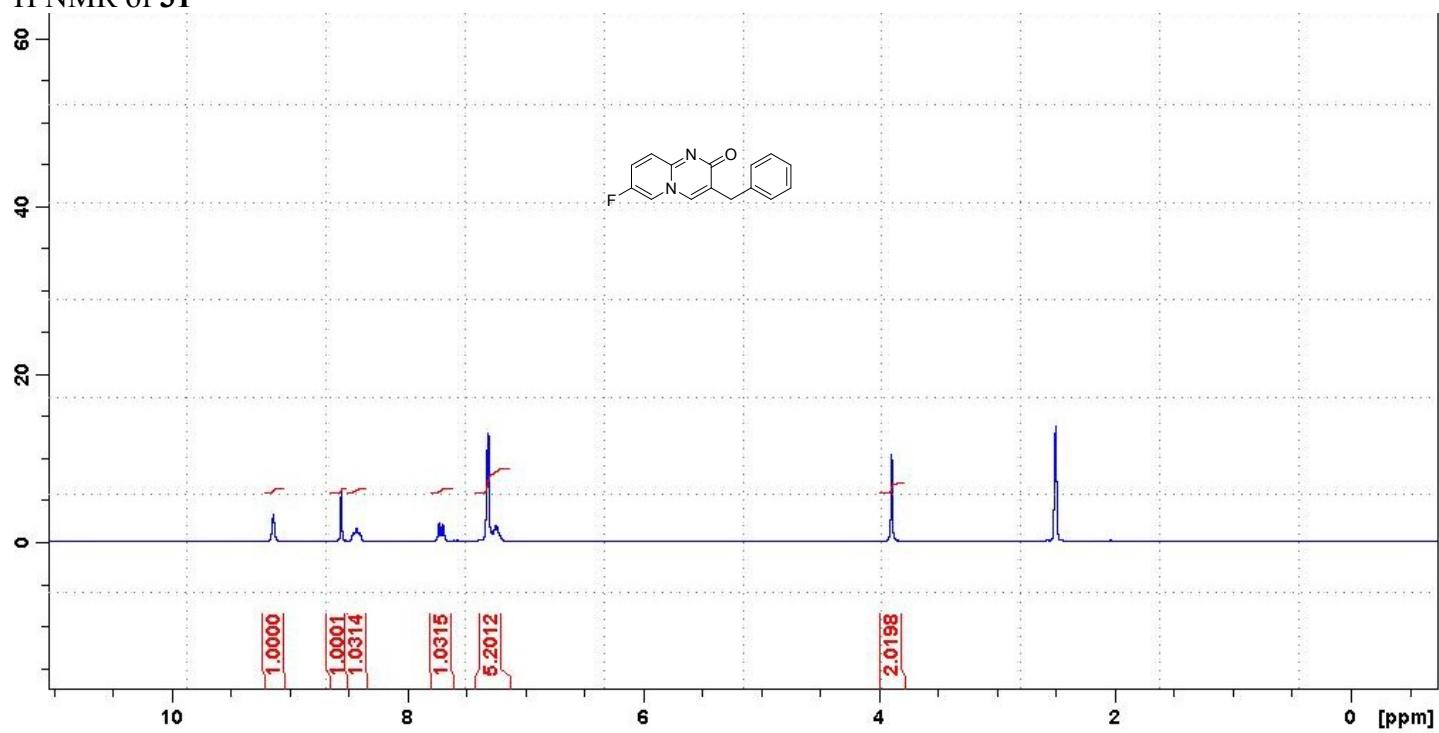


¹³C NMR of **30**

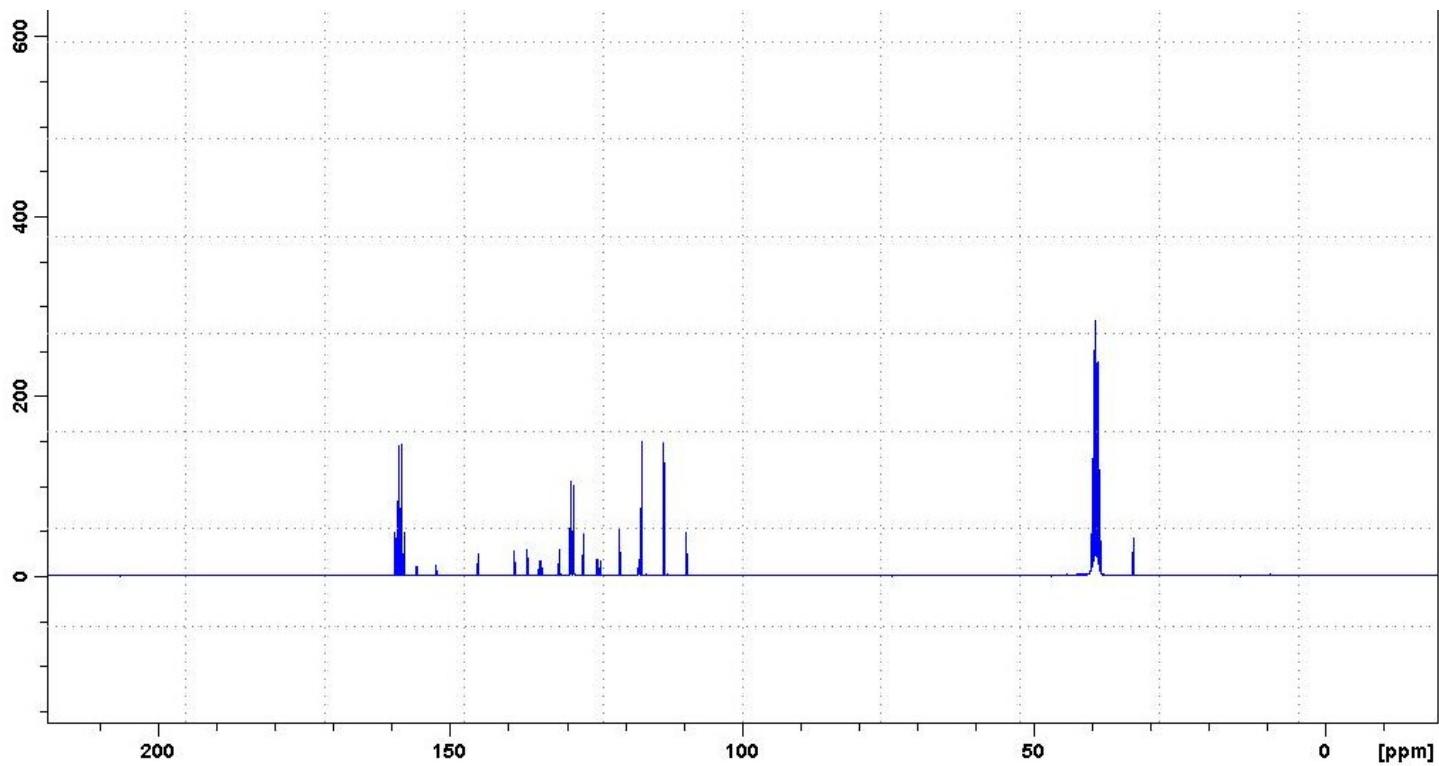


3-Benzyl-7-fluoro-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (31)

¹H NMR of 31

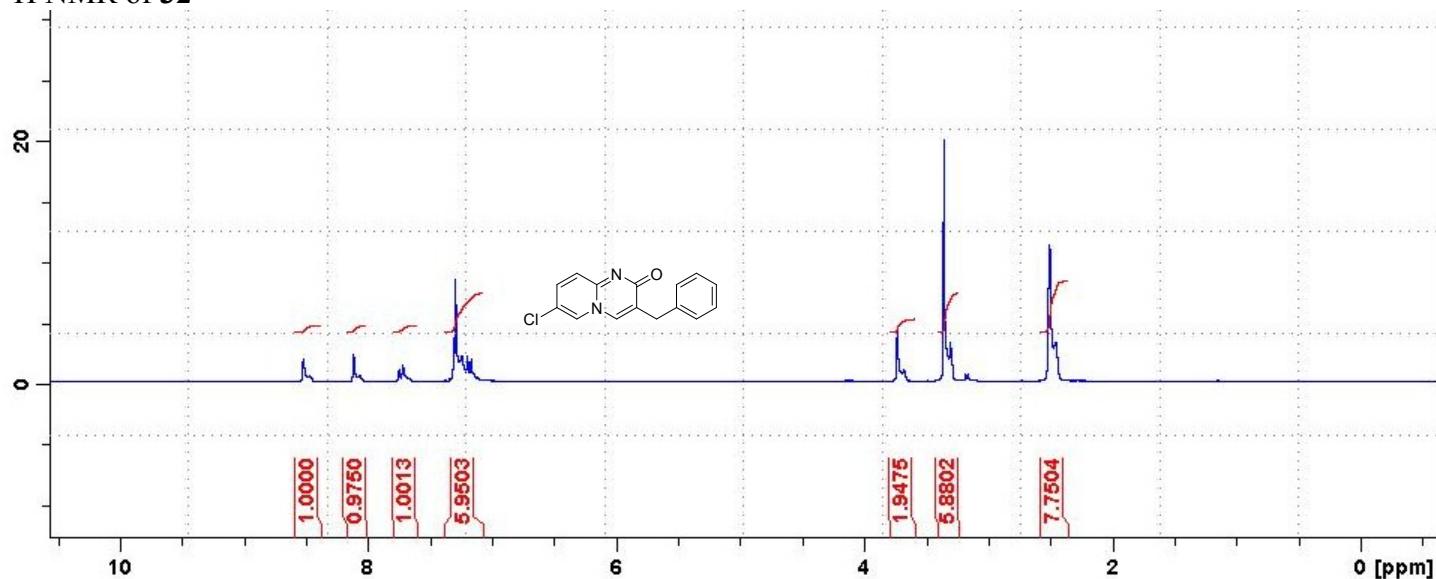


¹³C NMR of 31

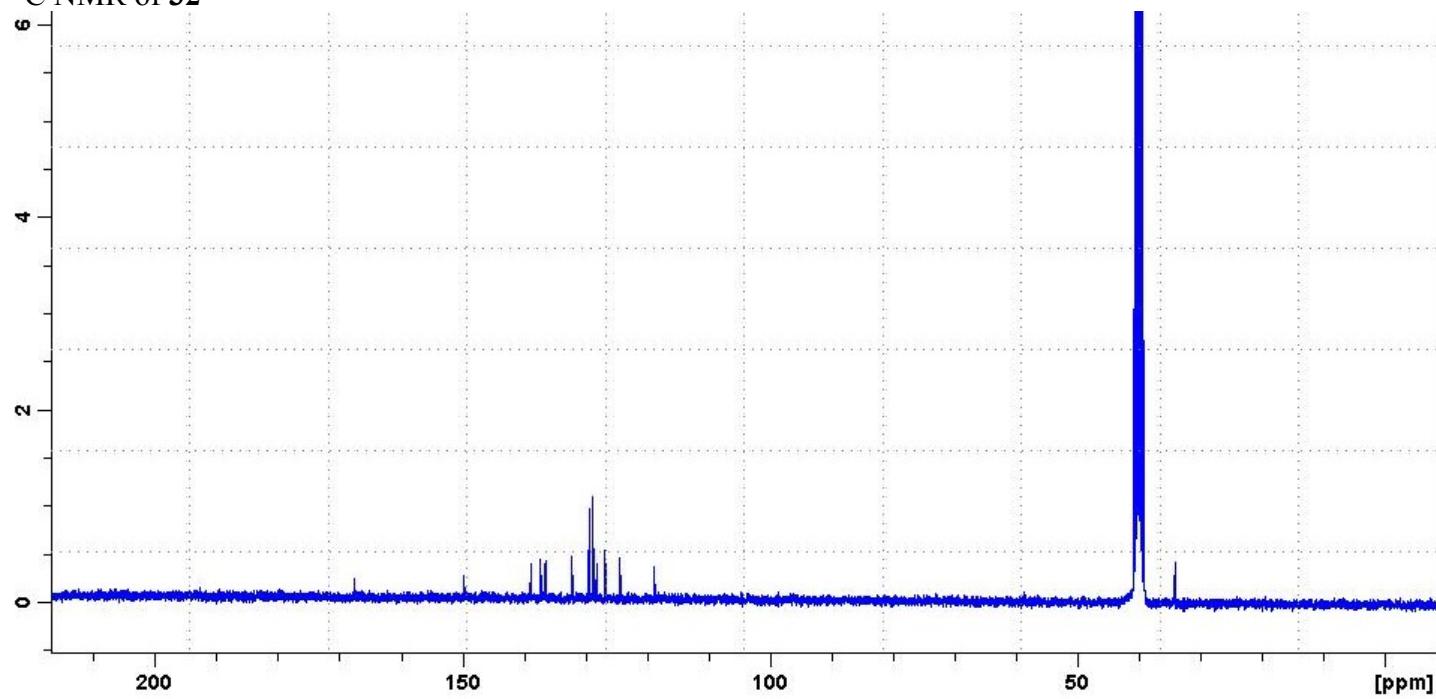


3-Benzyl-7-chloro-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (32)

¹H NMR of 32

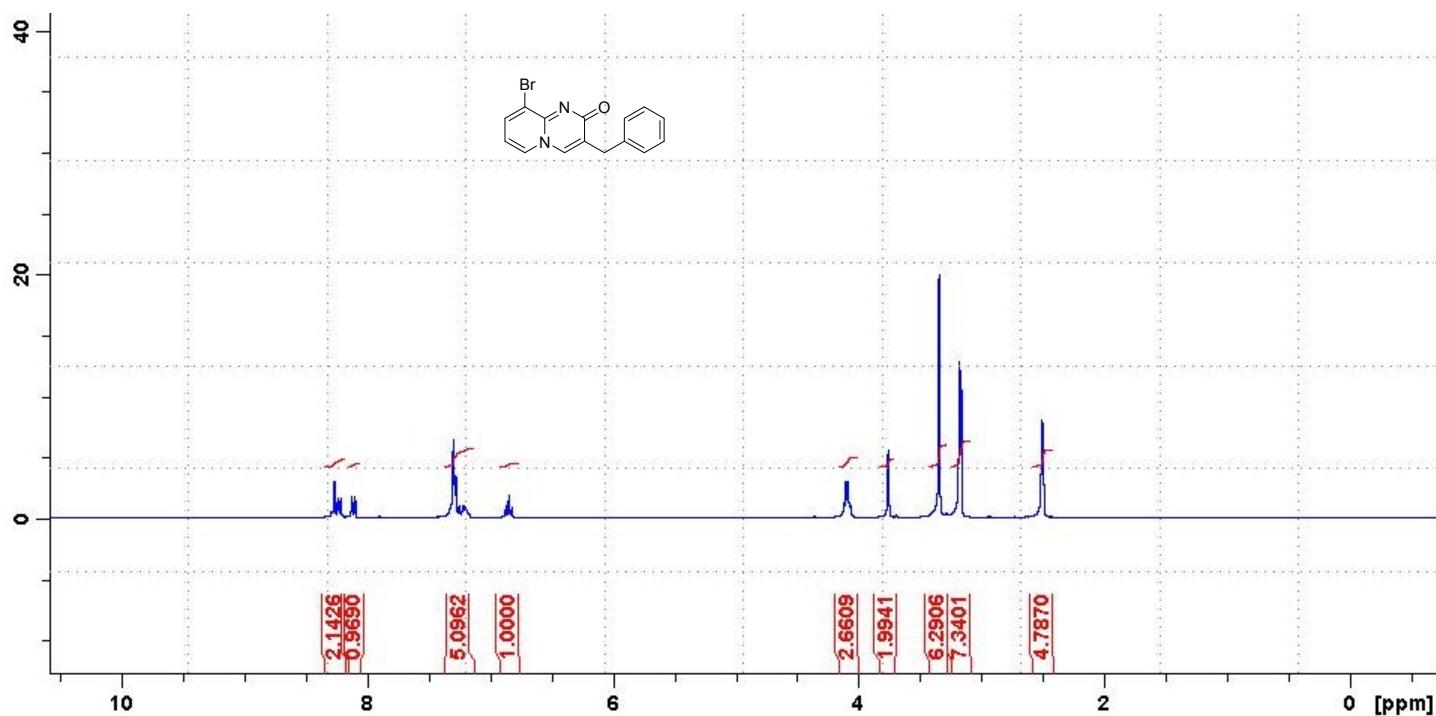


¹³C NMR of 32

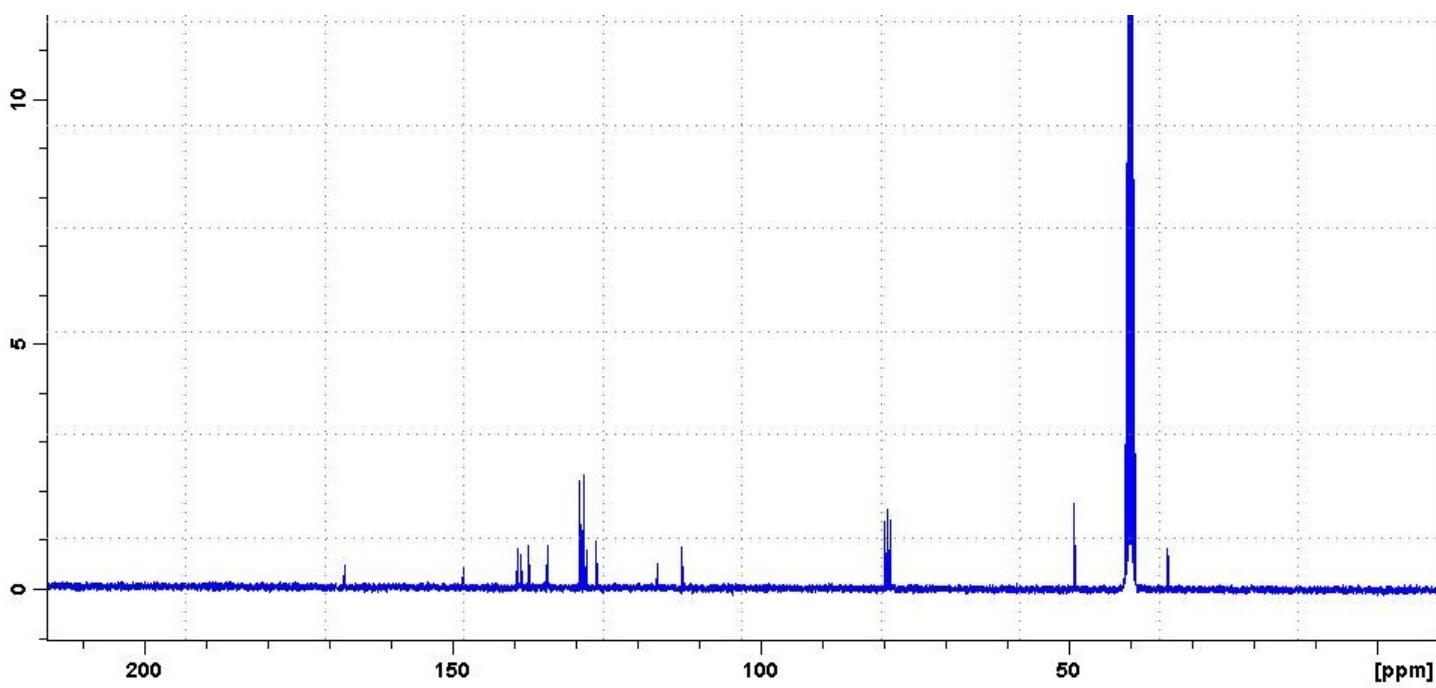


3-Benzyl-9-bromo-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (33)

¹H NMR of 33

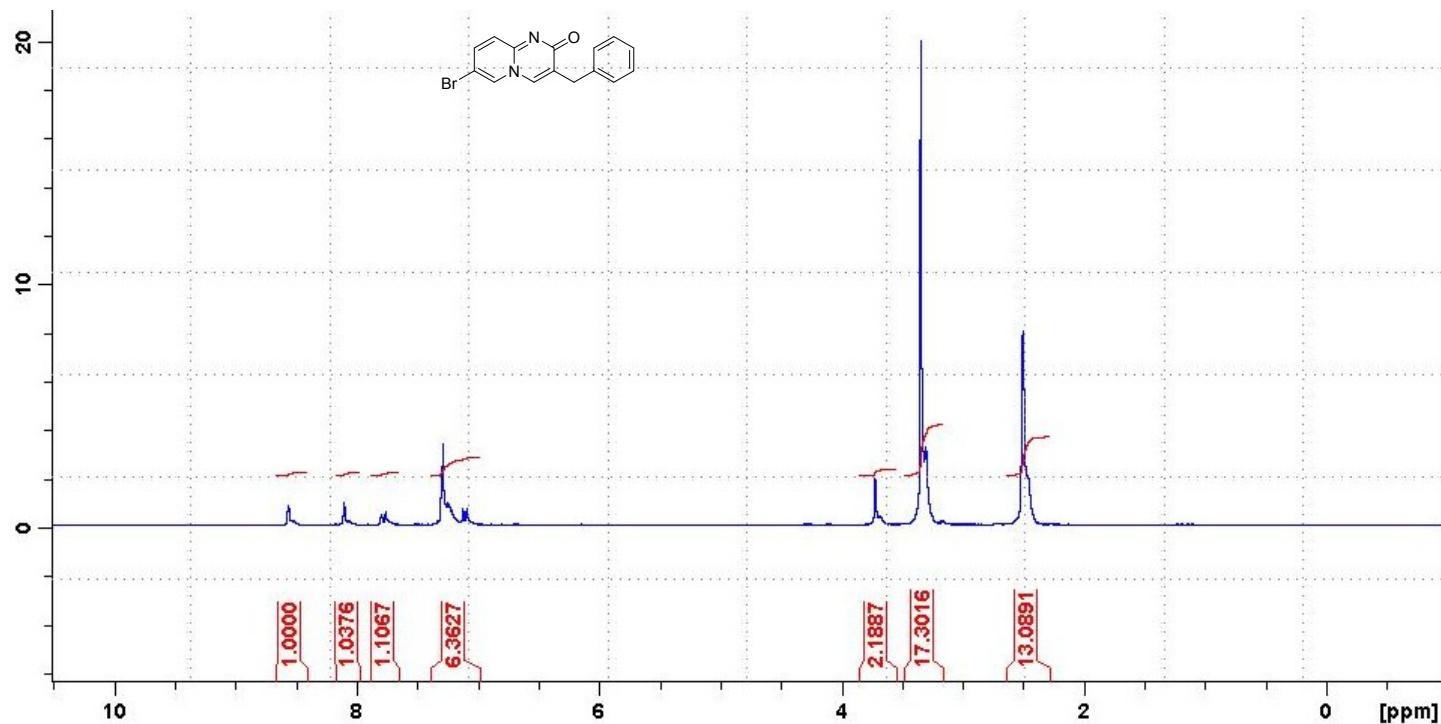


¹³C NMR of 33

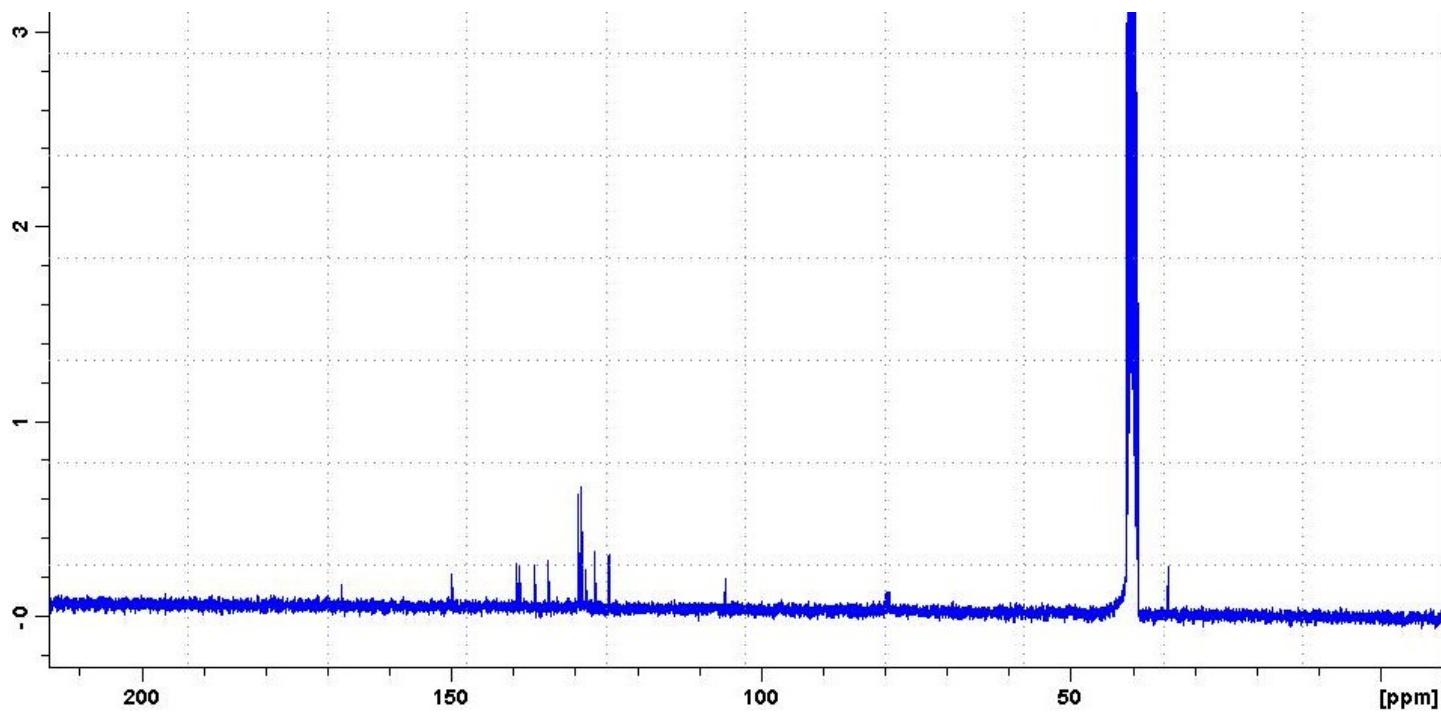


3-Benzyl-7-bromo-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (34)

¹H NMR of 34

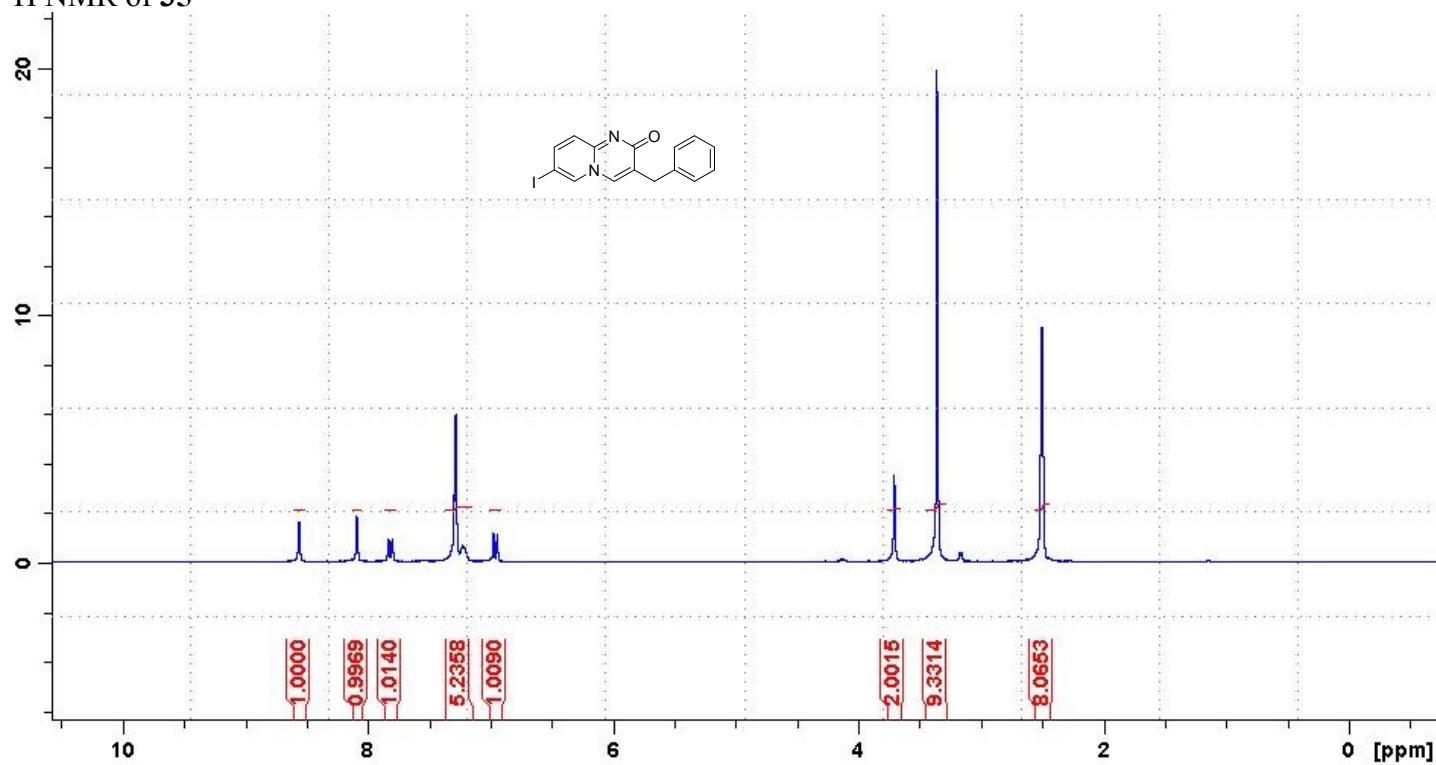


¹³C NMR of 34

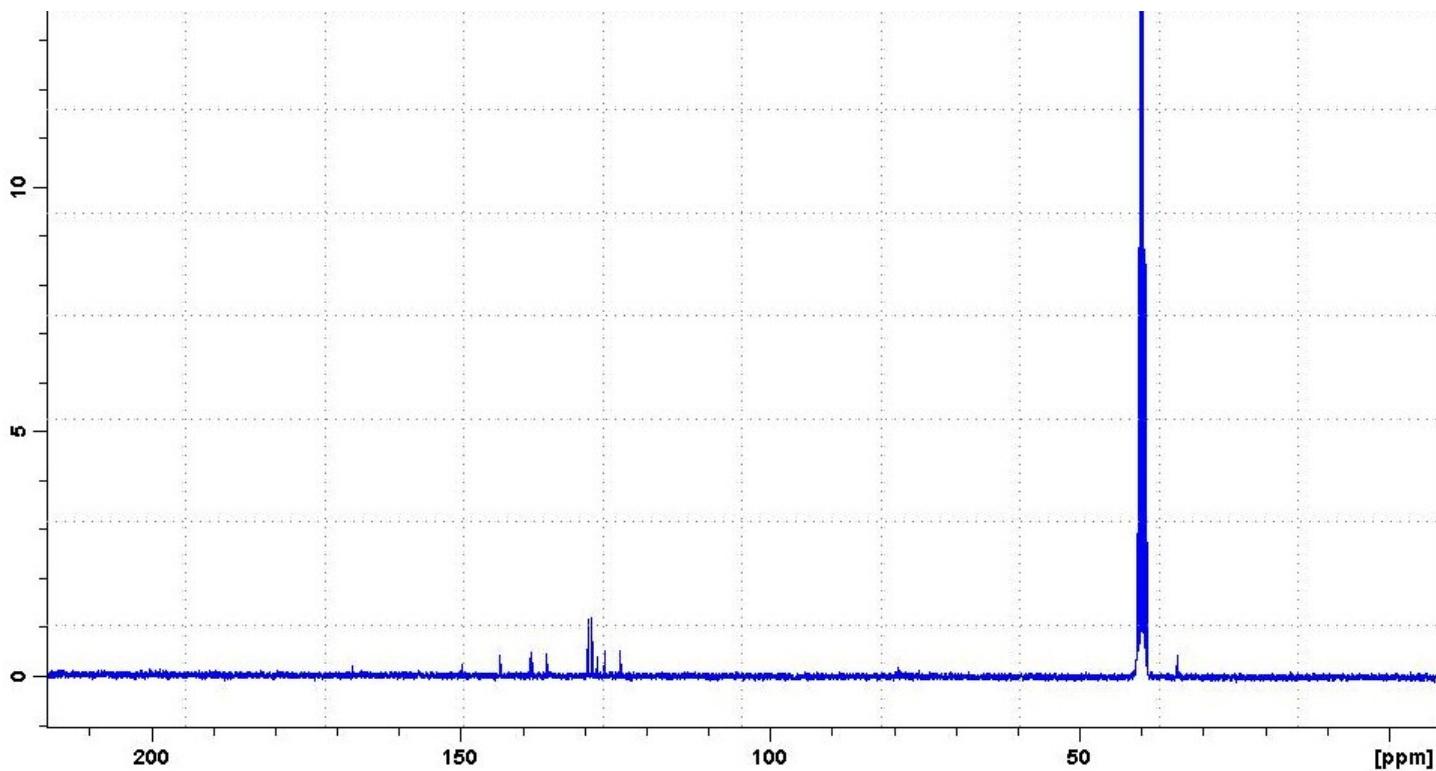


3-Benzyl-7-iodo-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (35)

¹H NMR of 35

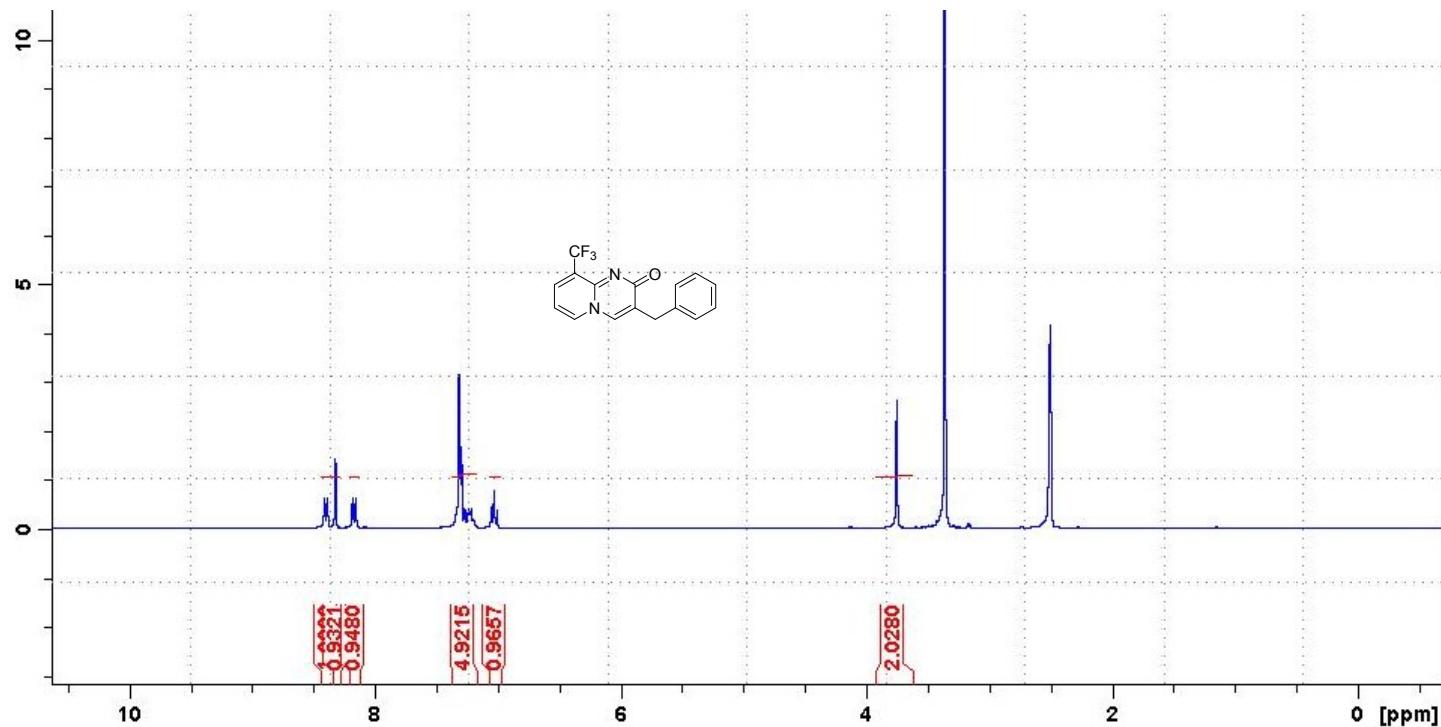


¹³C NMR of 35

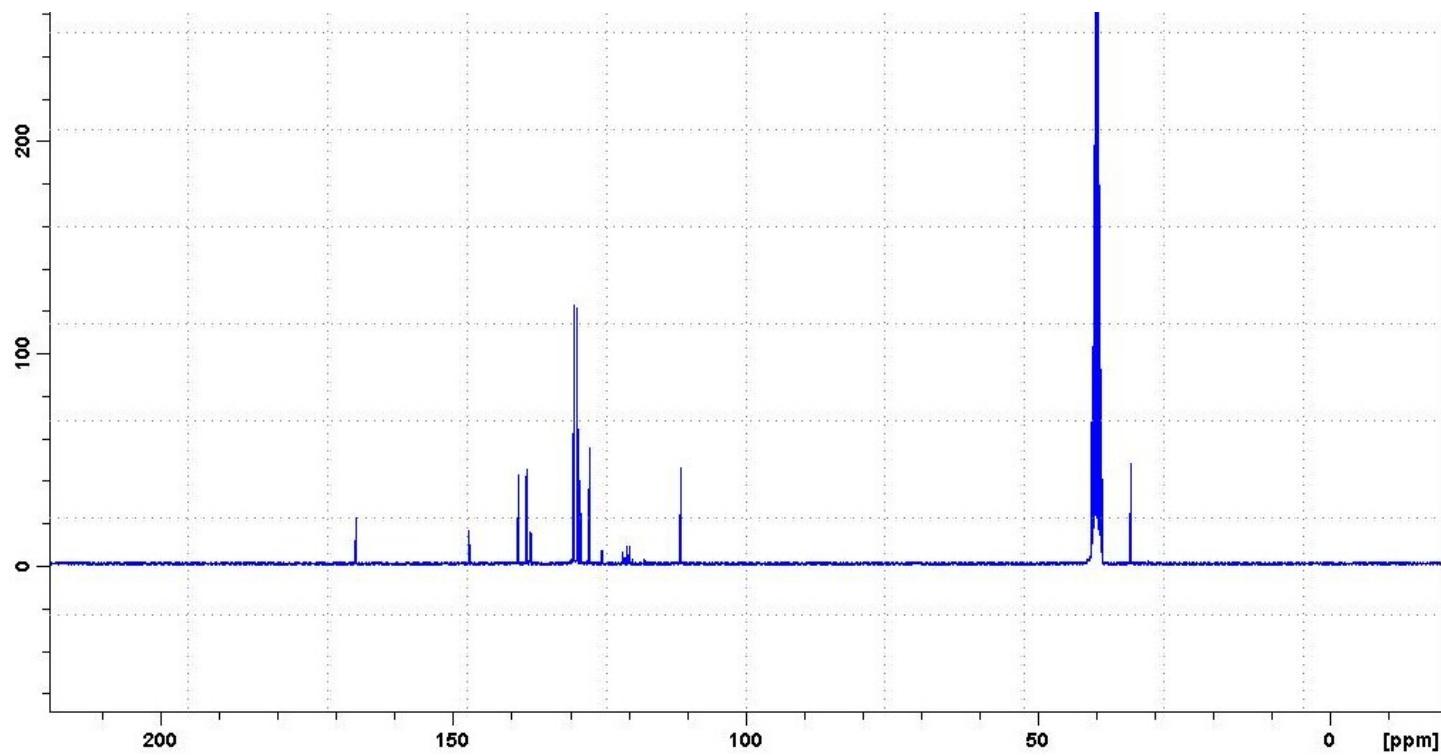


3-(Benzyl)-9-(trifluoromethyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (36)

¹H NMR of 36

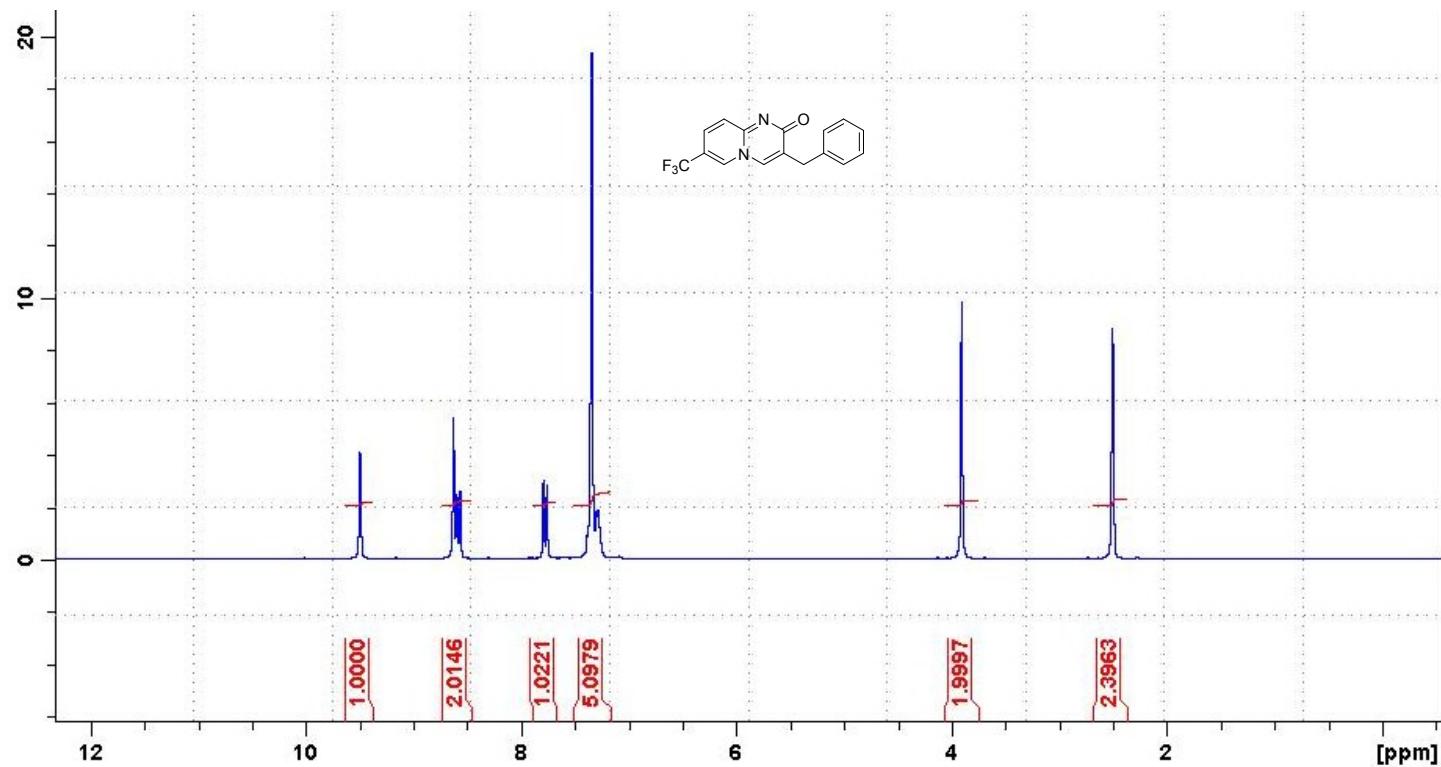


¹³C NMR of 36

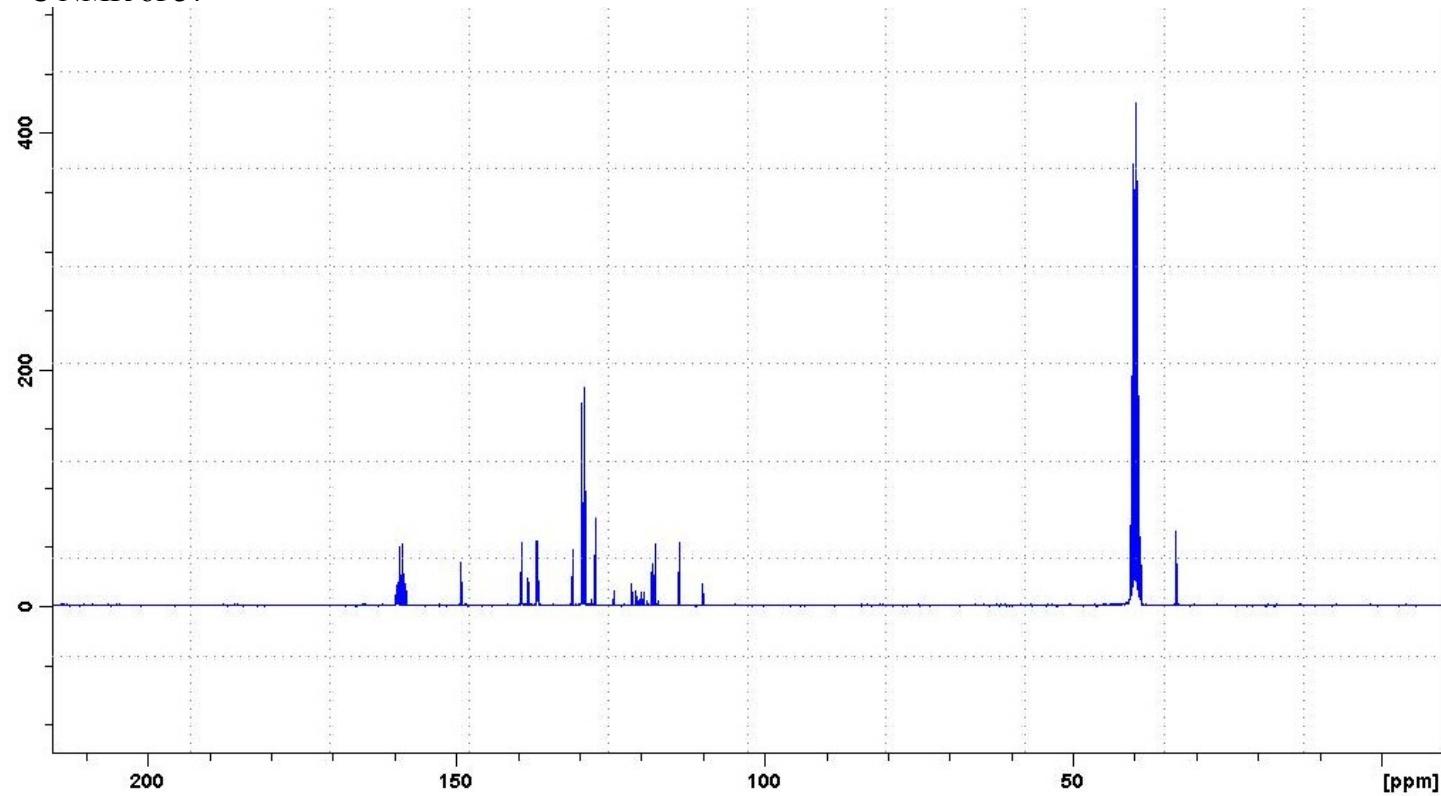


3-Benzyl-7-(trifluoromethyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (37)

¹H NMR of 37

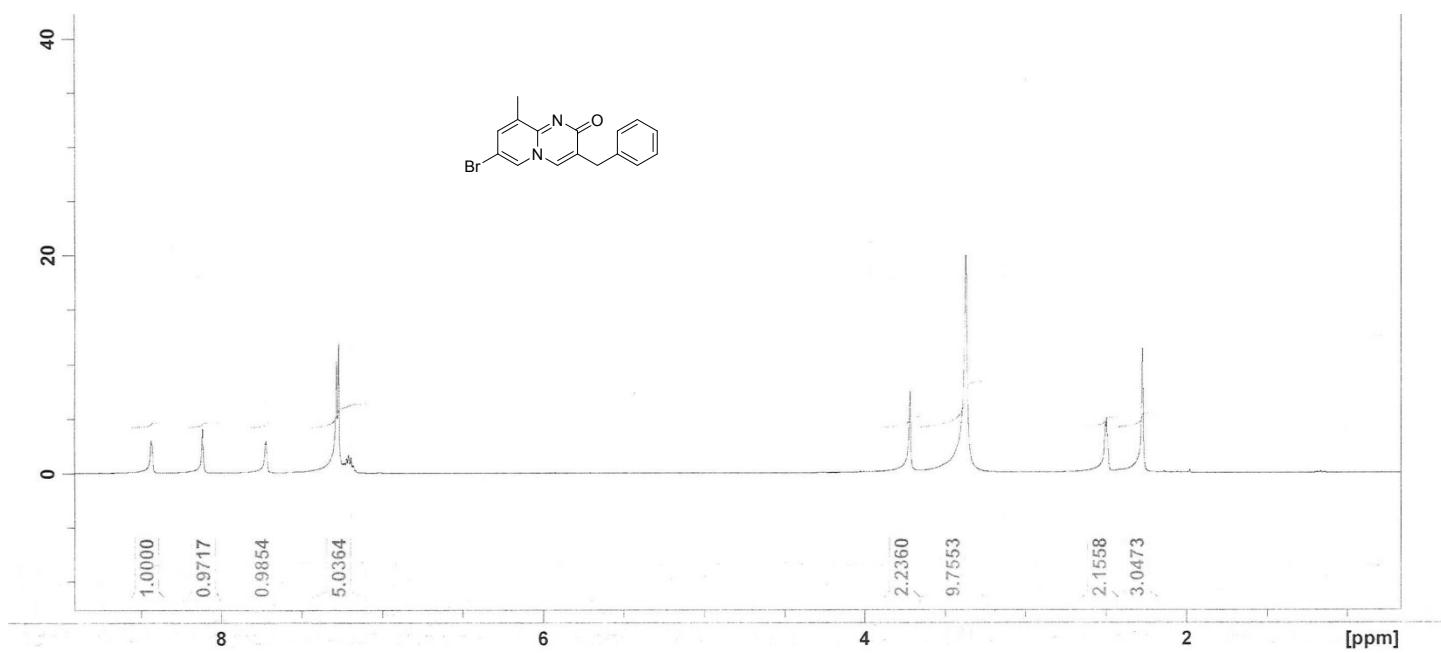


¹³C NMR of 37

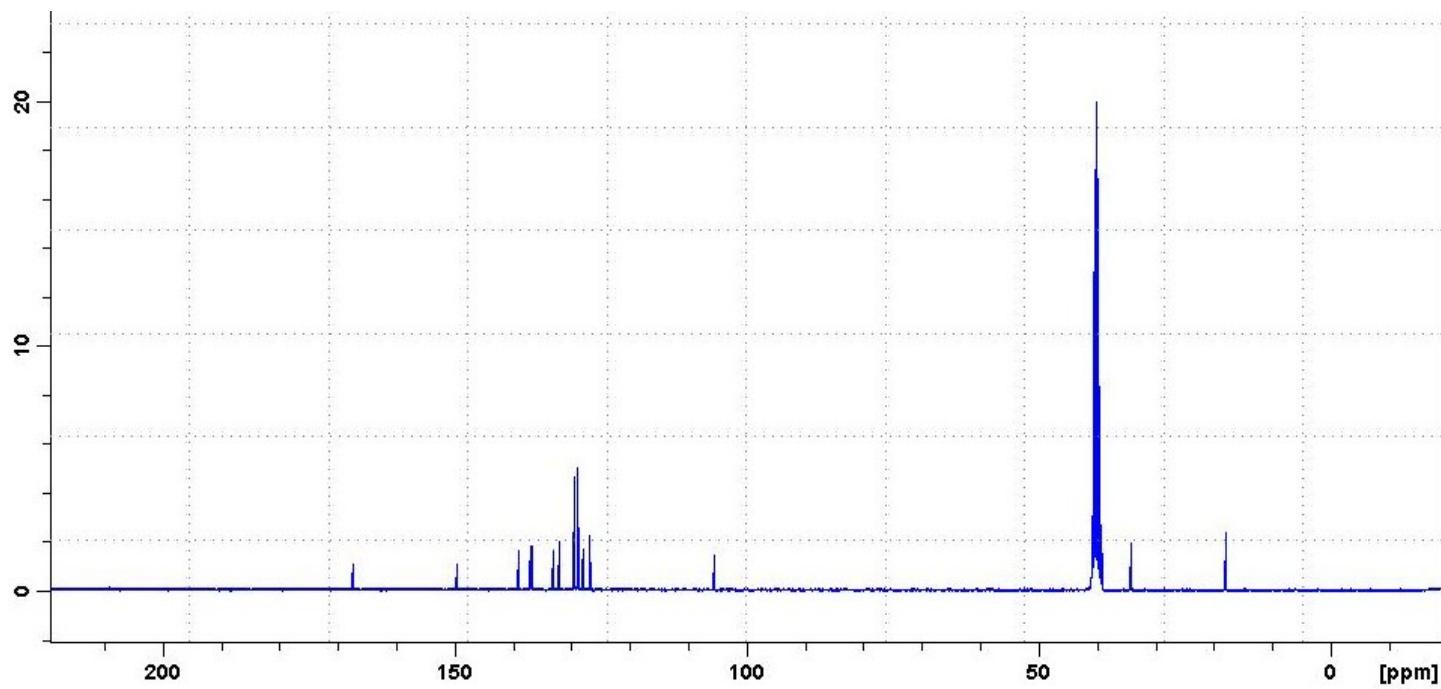


3-Benzyl-7-bromo-9-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (38)

¹H NMR of **38**

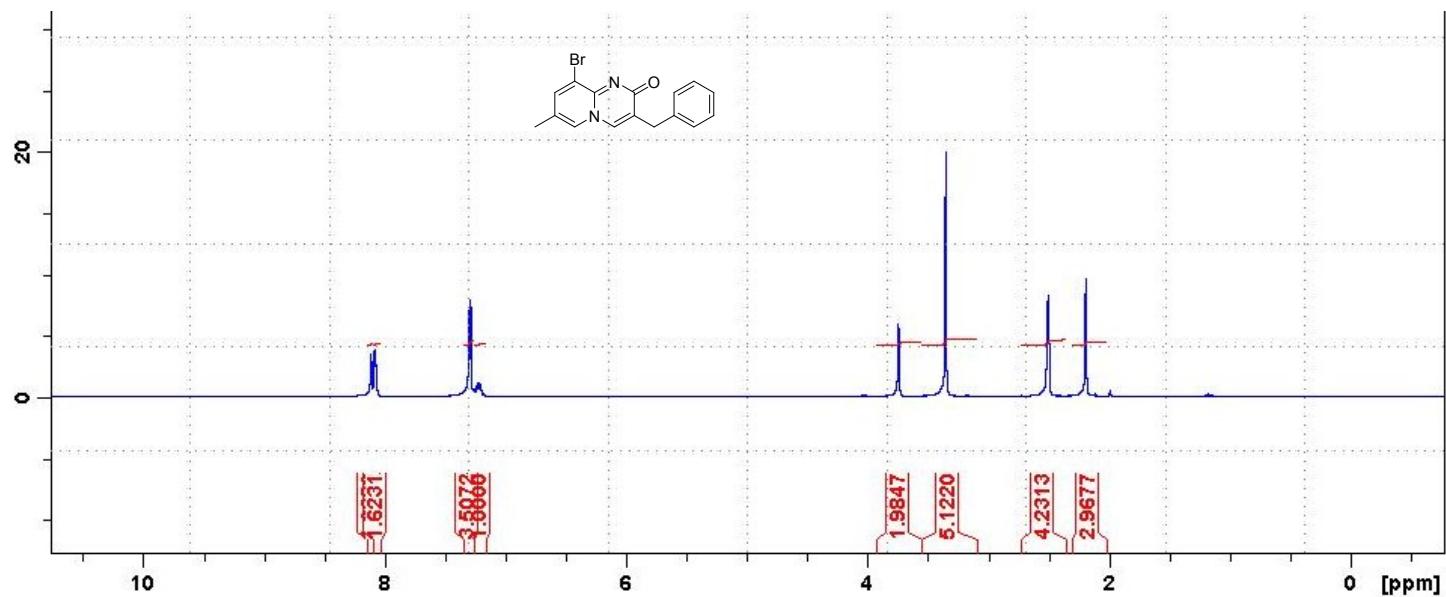


¹³C NMR of **38**

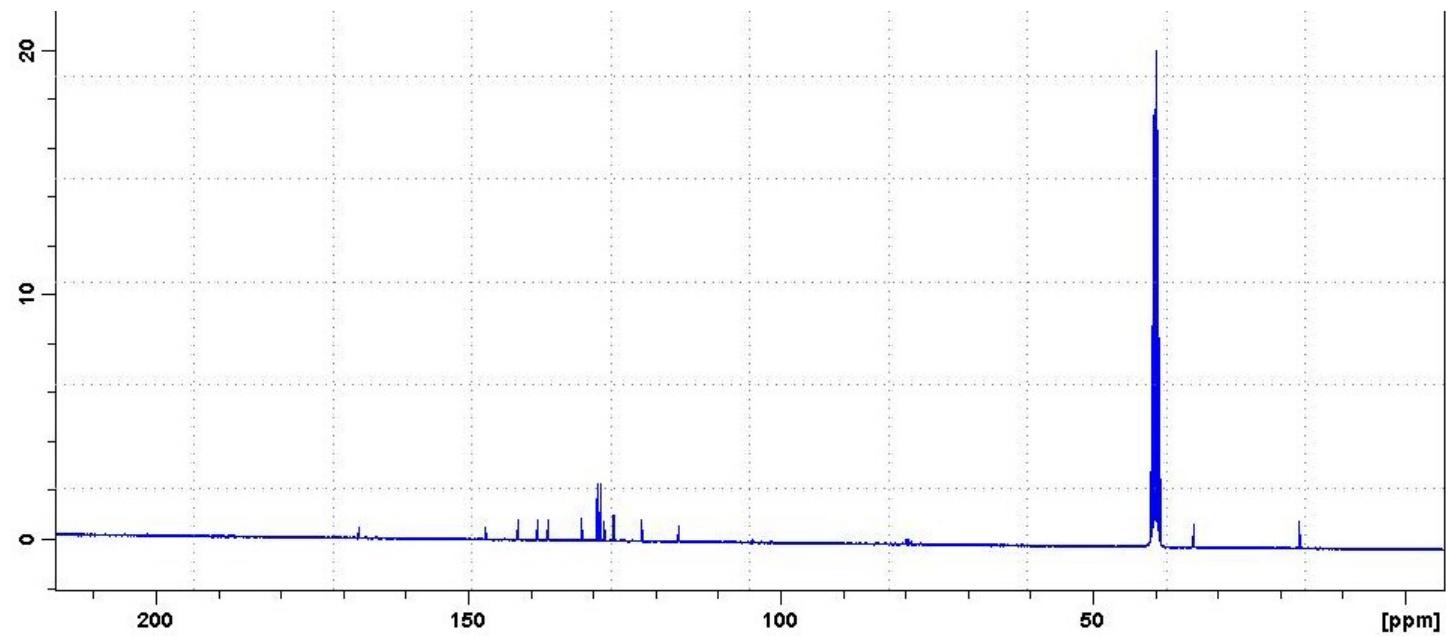


3-Benzyl-9-bromo-7-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (39)

¹H NMR of 39

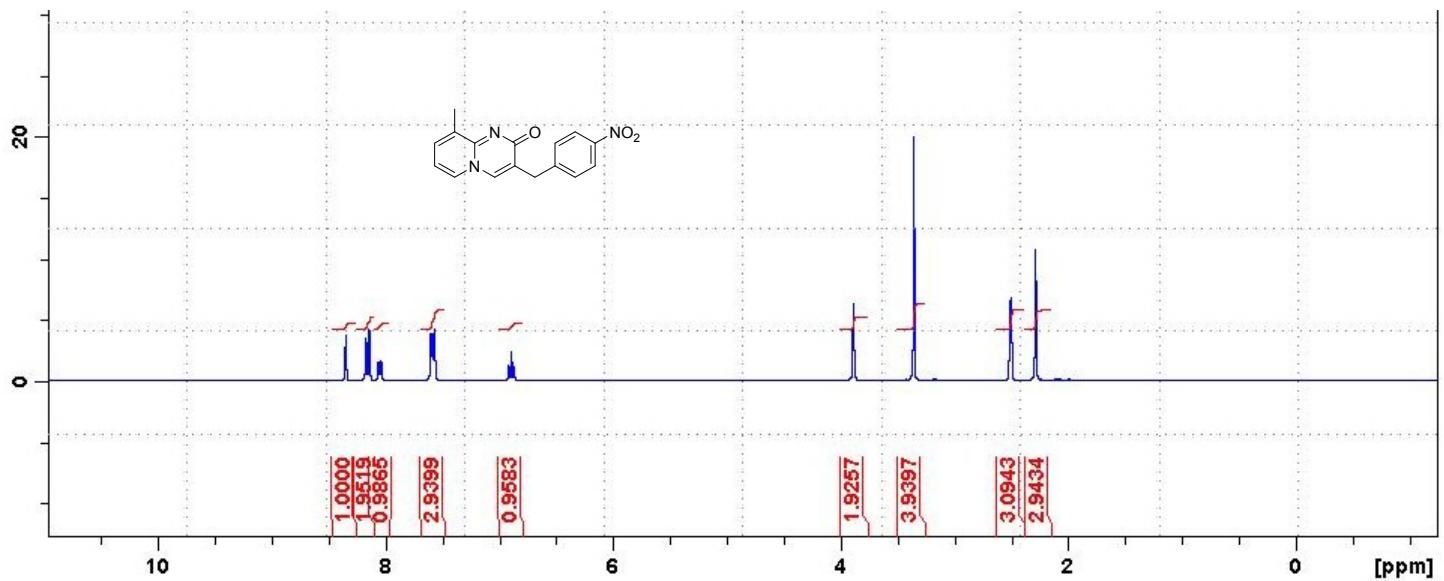


¹³C NMR of 39

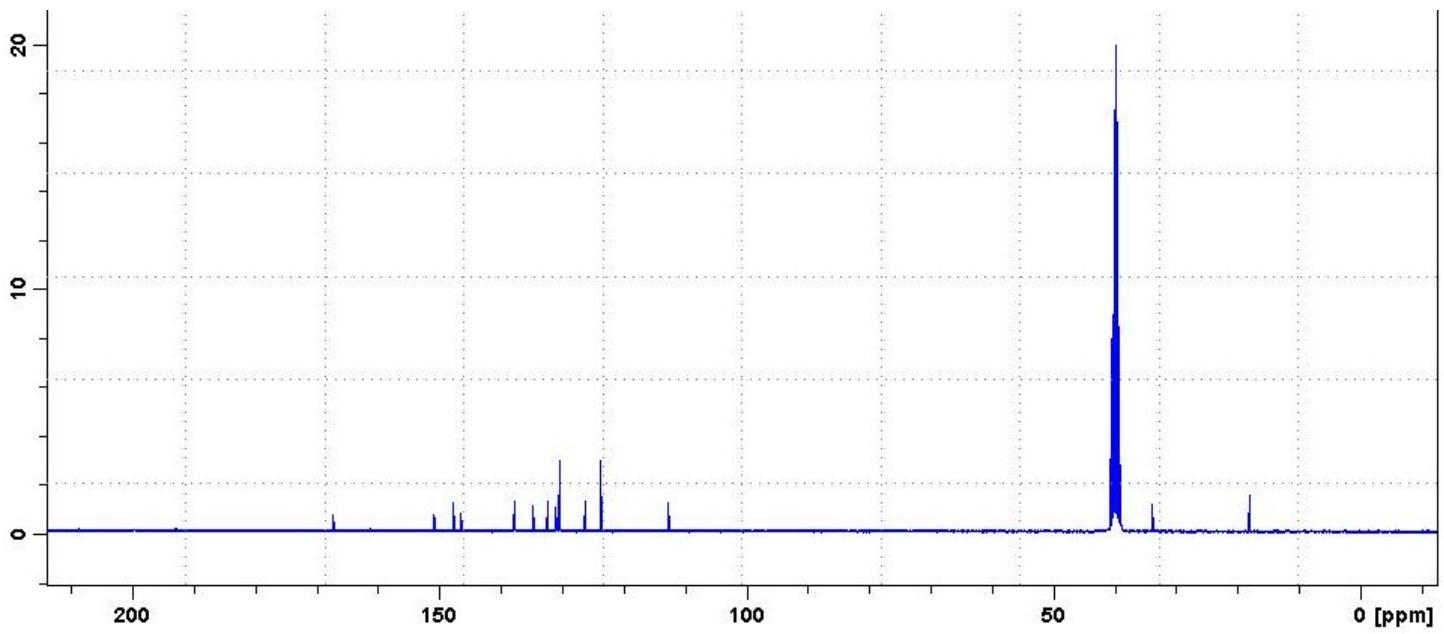


9-Methyl-3-[(4-nitrophenyl)methyl]-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (40**)**

¹H NMR of **40**

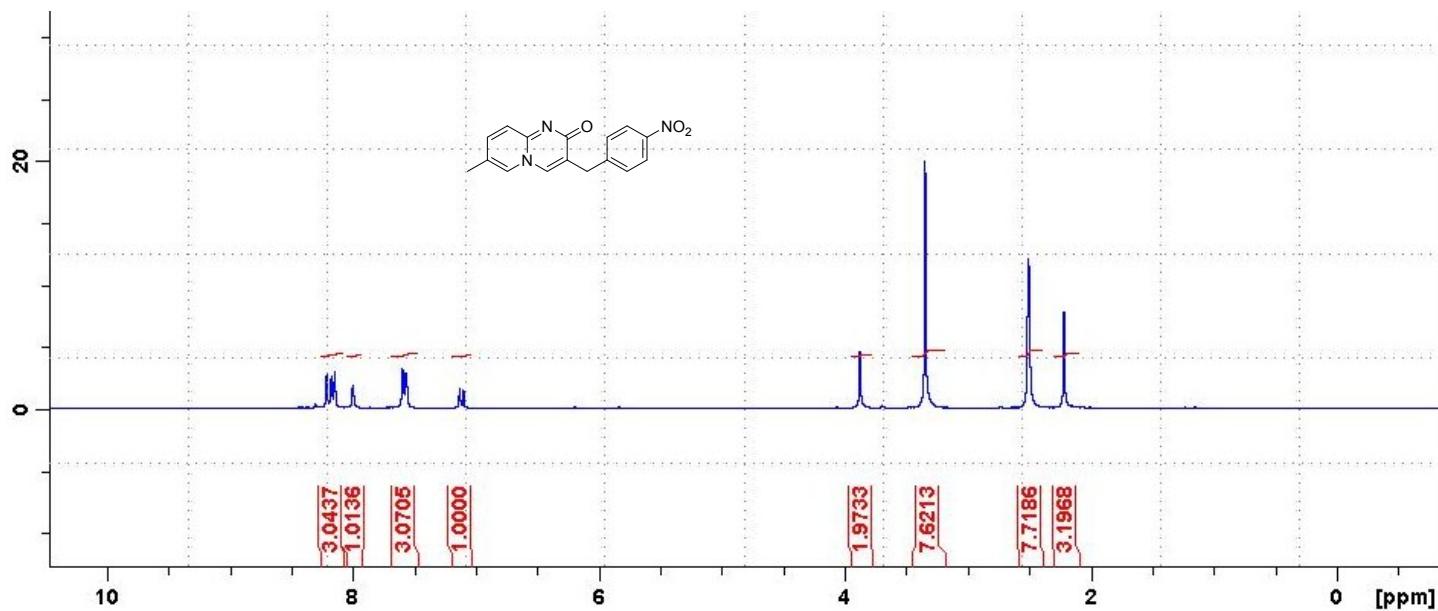


¹³C NMR of **40**

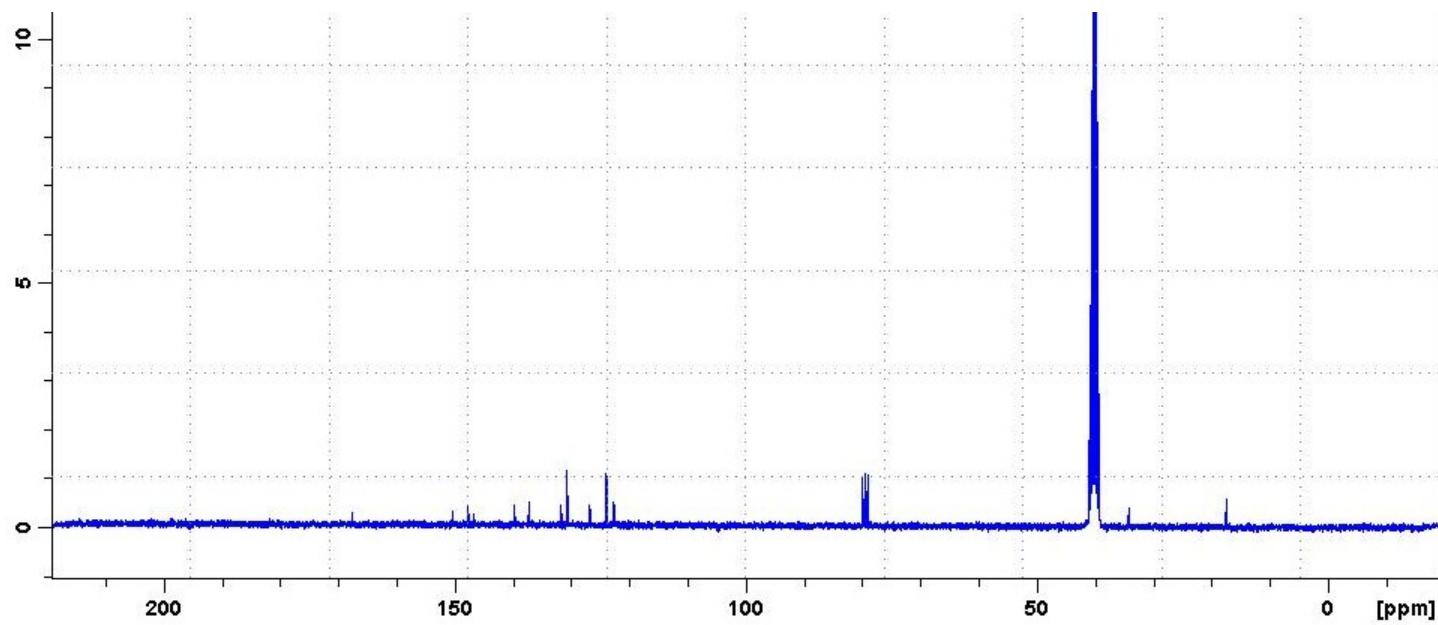


7-Methyl-3-[(4-nitrophenyl)methyl]-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (41)

¹H NMR of 41

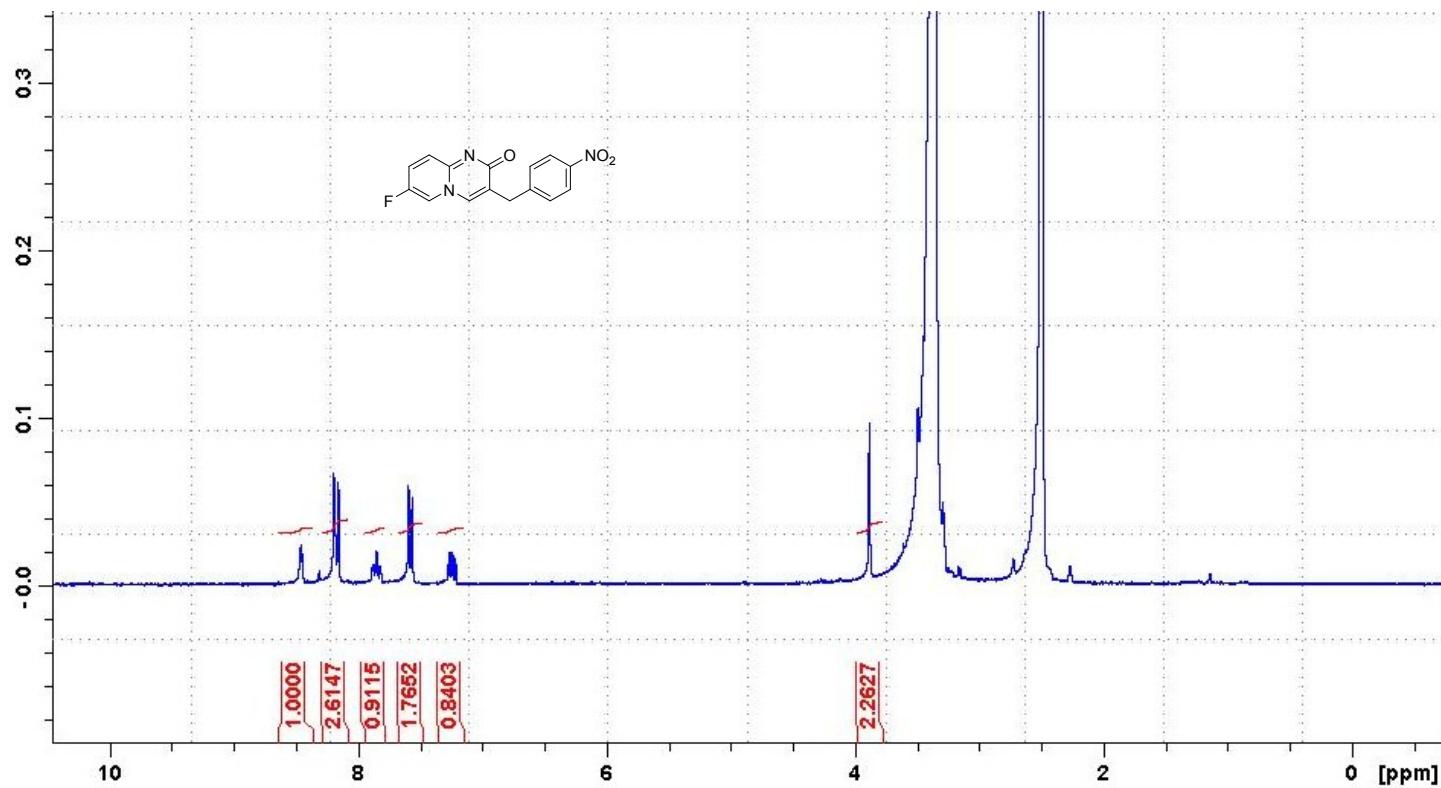


¹³C NMR of 41

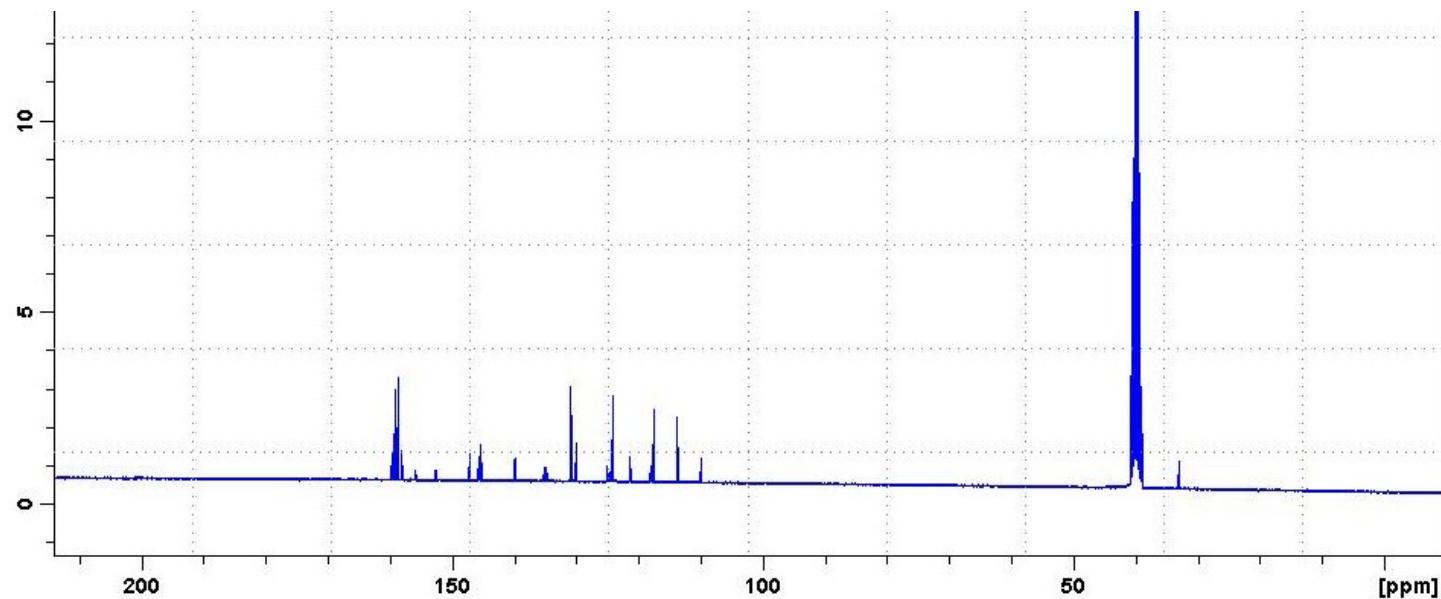


7-Fluoro-3-(4-nitrobenzyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (42)

¹H NMR of **42**

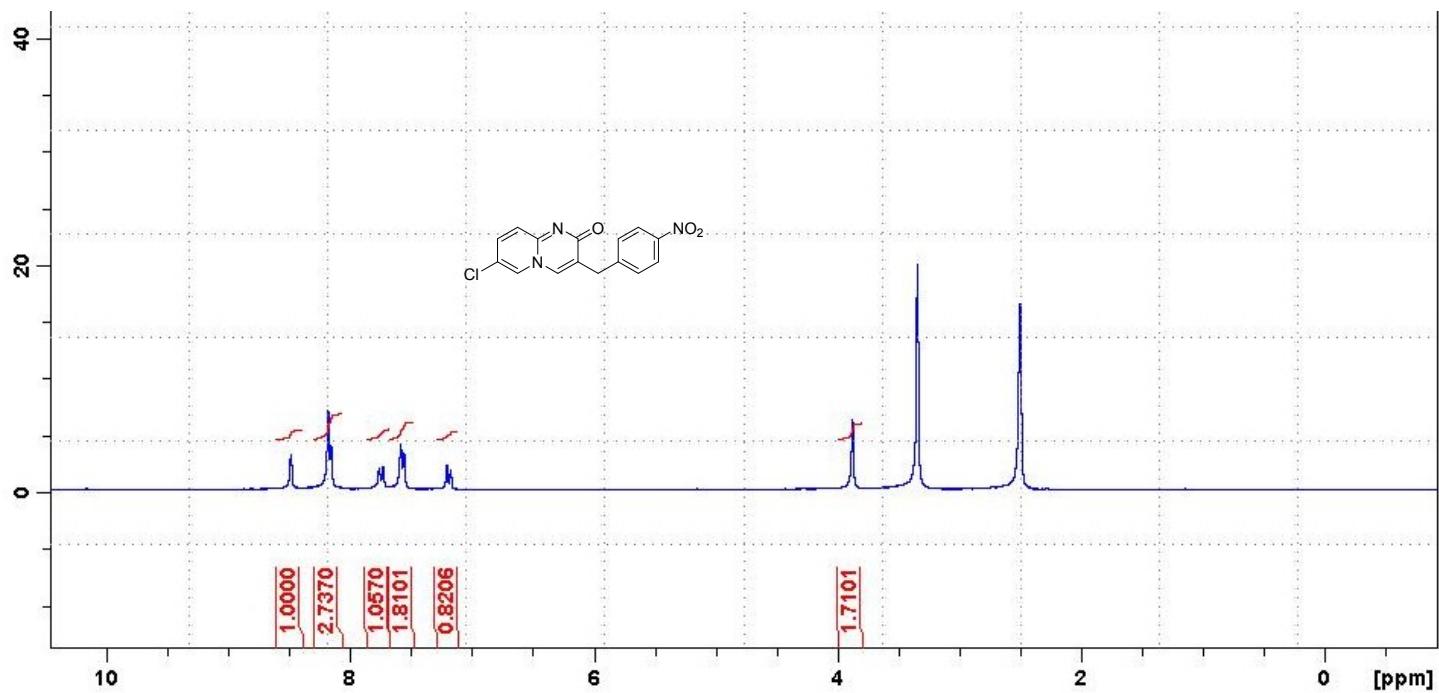


¹³C NMR of **42**

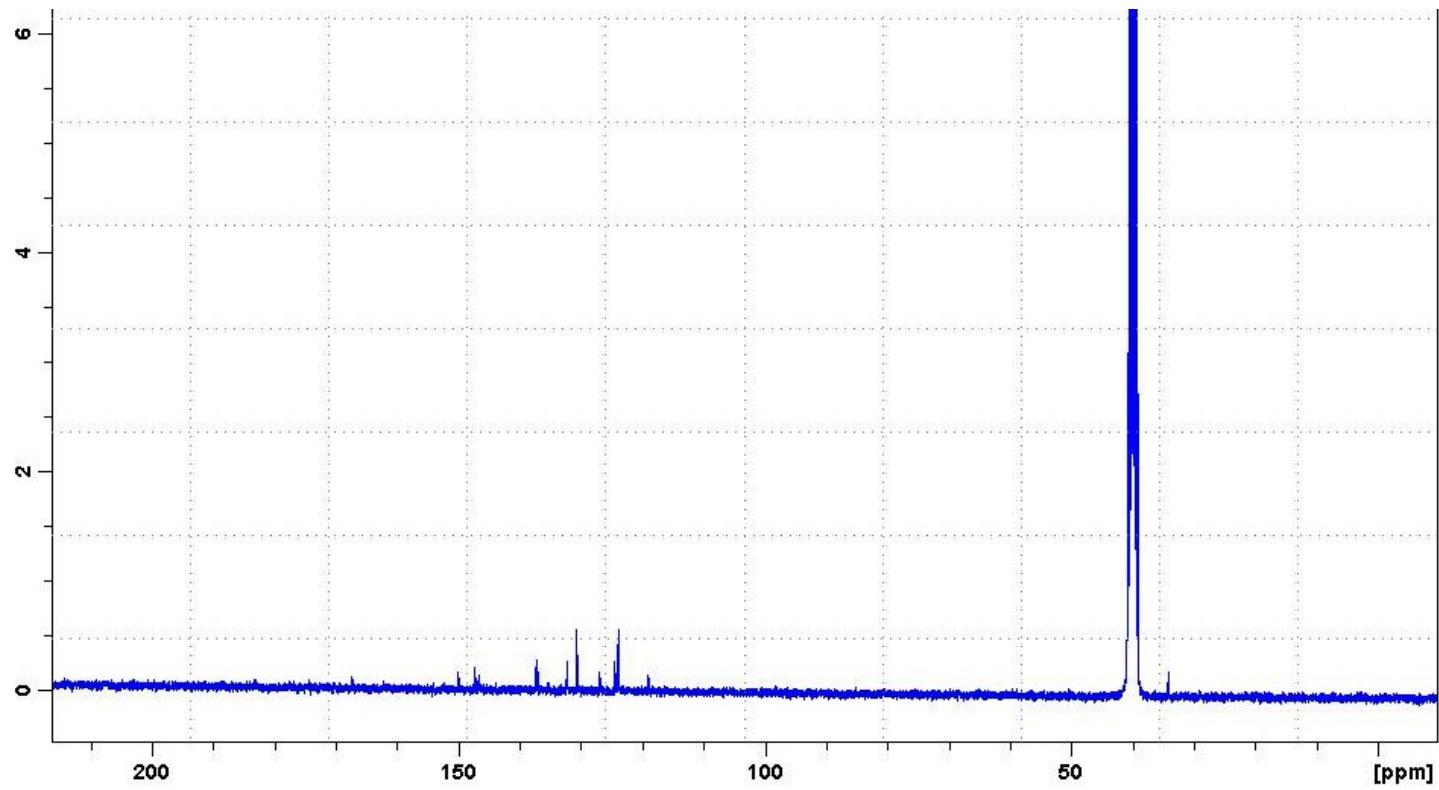


7-Chloro-3-(4-nitrobenzyl)-2*H*-pyrido[1,2-*a*]pyrimidin-2-one (43)

¹H NMR of 43

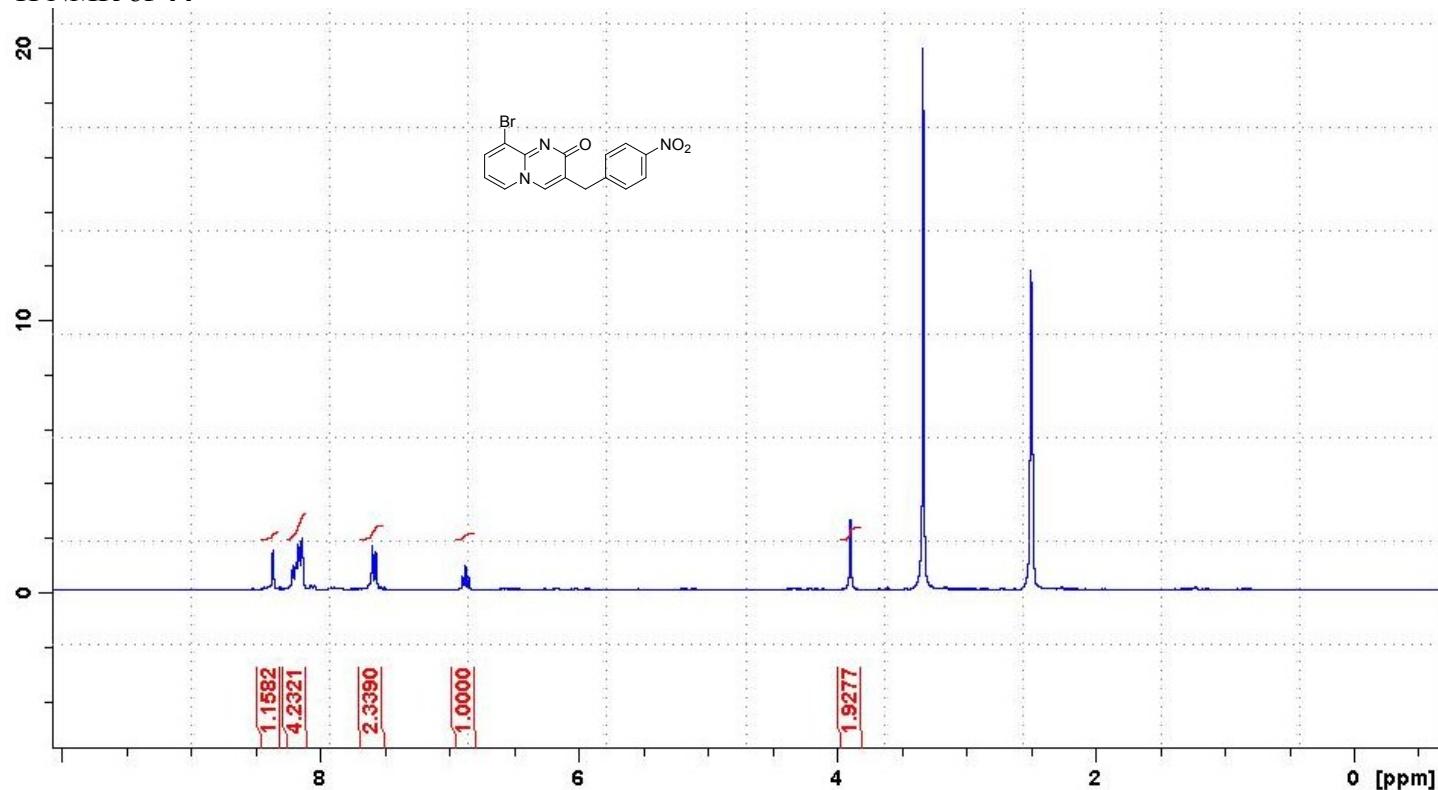


¹³C NMR of 43

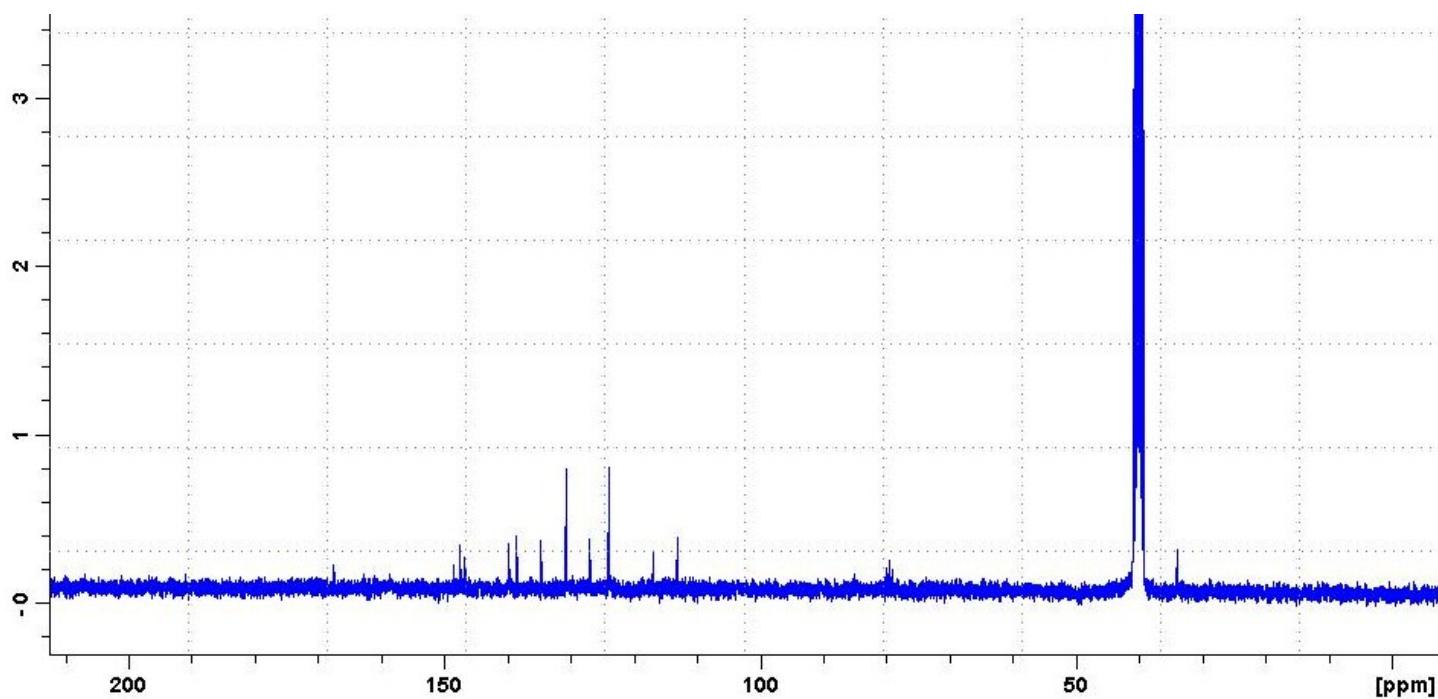


9-Bromo-3-[(4-nitrophenyl)methyl]-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (44)

¹H NMR of 44

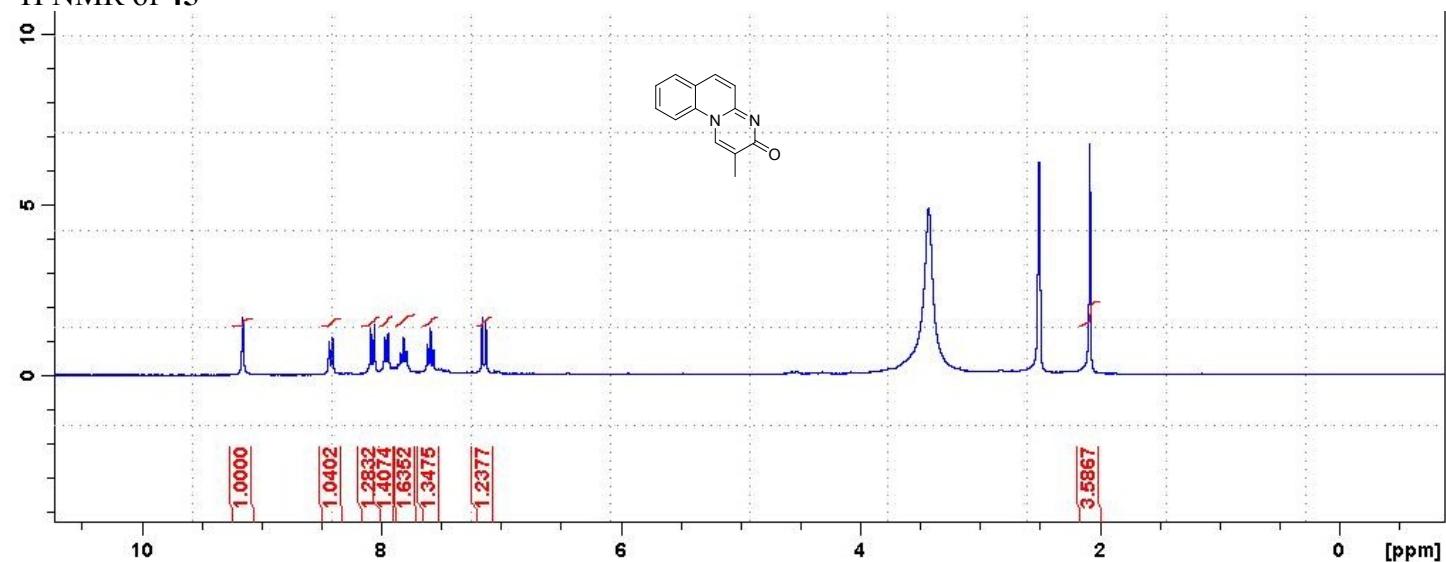


¹³C NMR of 44



2-Methyl-3H-pyrimido[1,2-a]quinolin-3-one (45)

¹H NMR of **45**



¹³C NMR of **45**

