SUPPORTING INFORMATION

In vitro and *in silico* studies on cytotoxic properties of oxythiamine and 2′-methylthiamine

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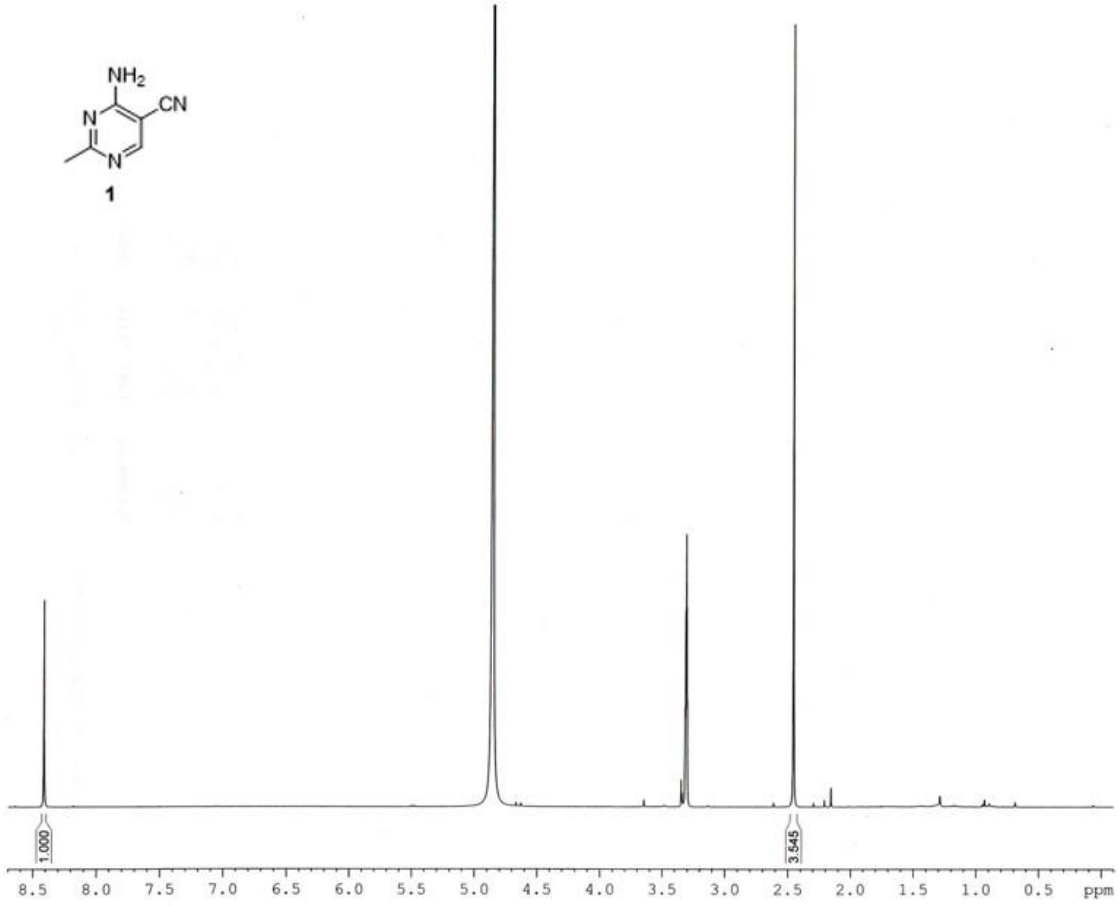
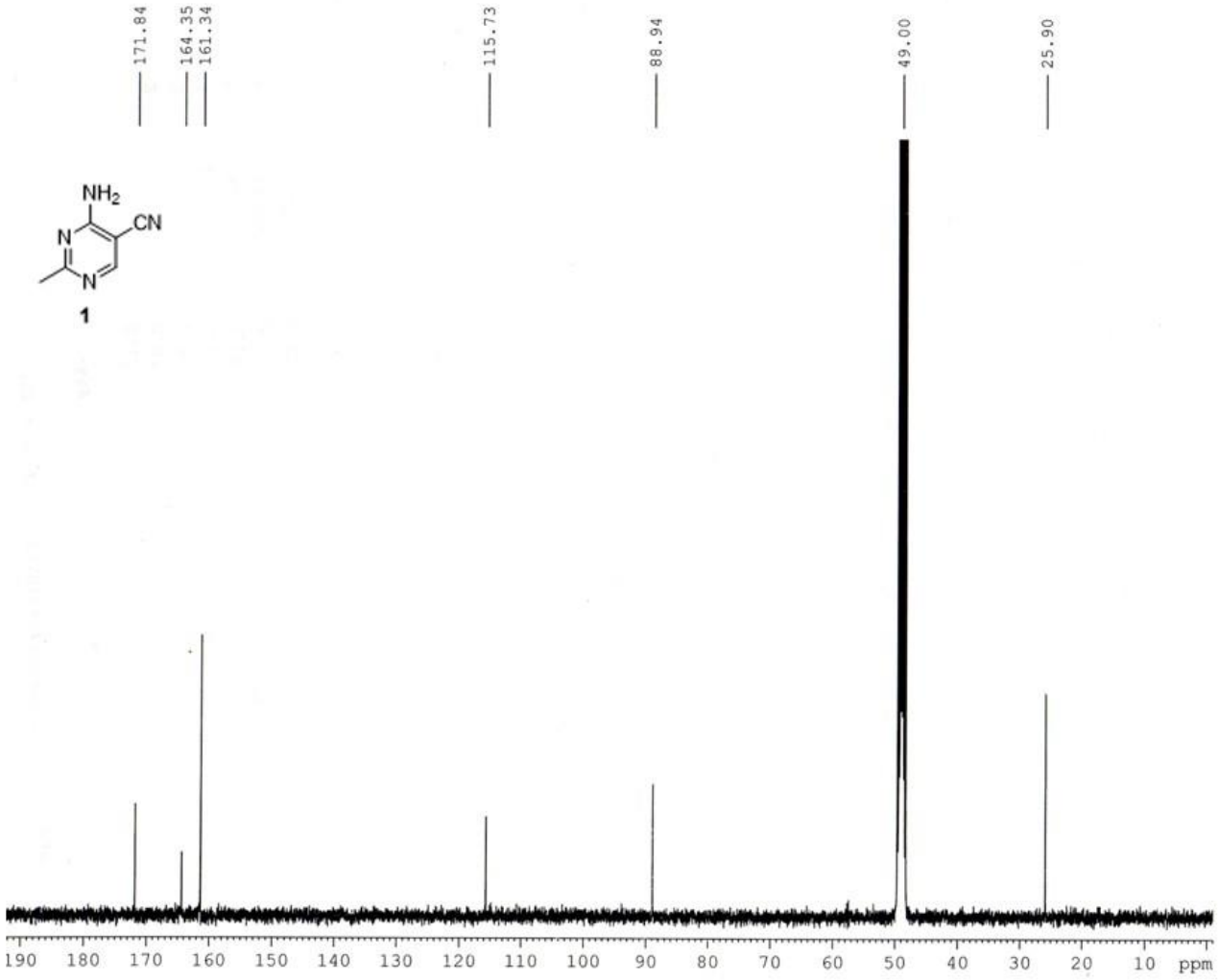
Copies of NMR spectra of new compounds

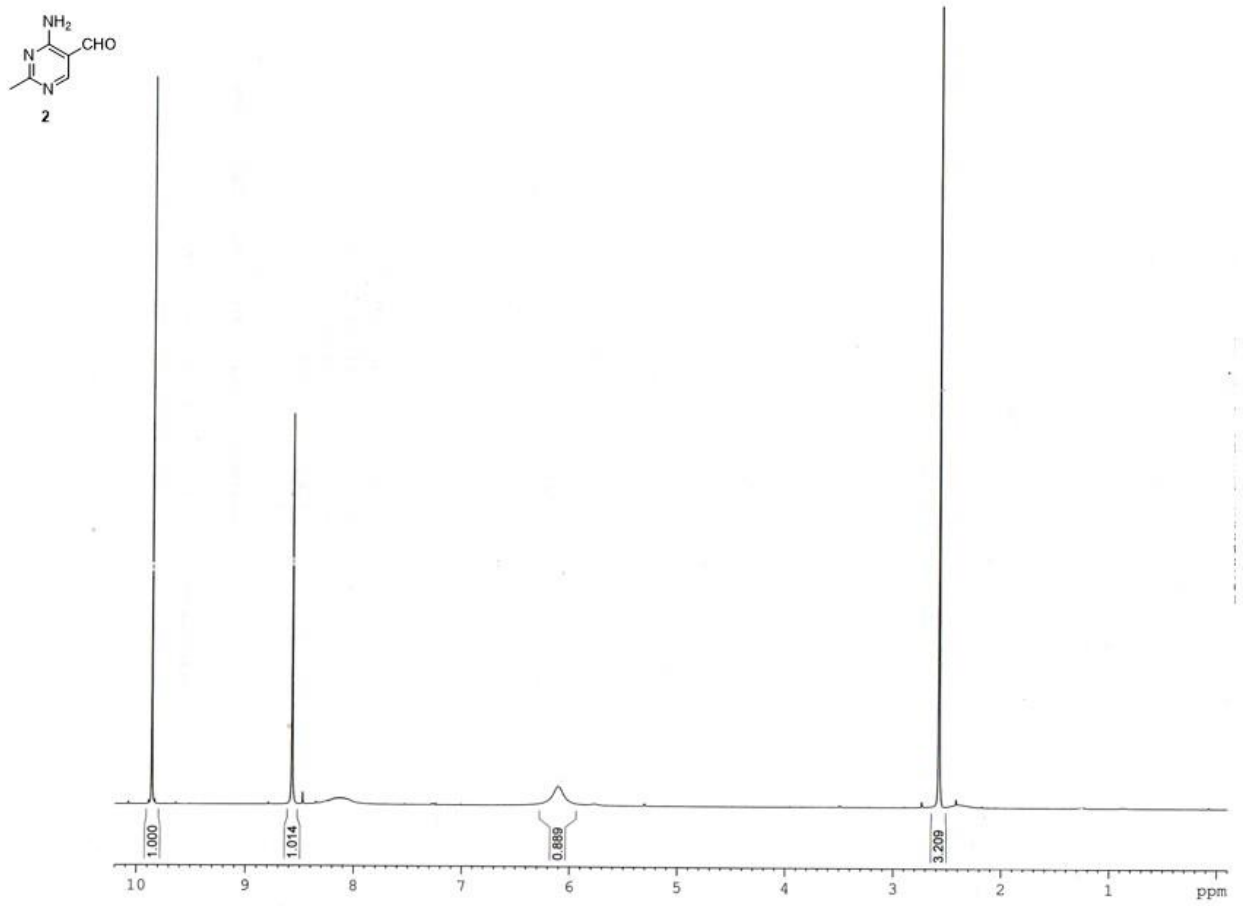
S1 – ^{1}H NMR spectrum of *4- Amino-2-methylpyrimidine- 5-carbonitrile (1)*



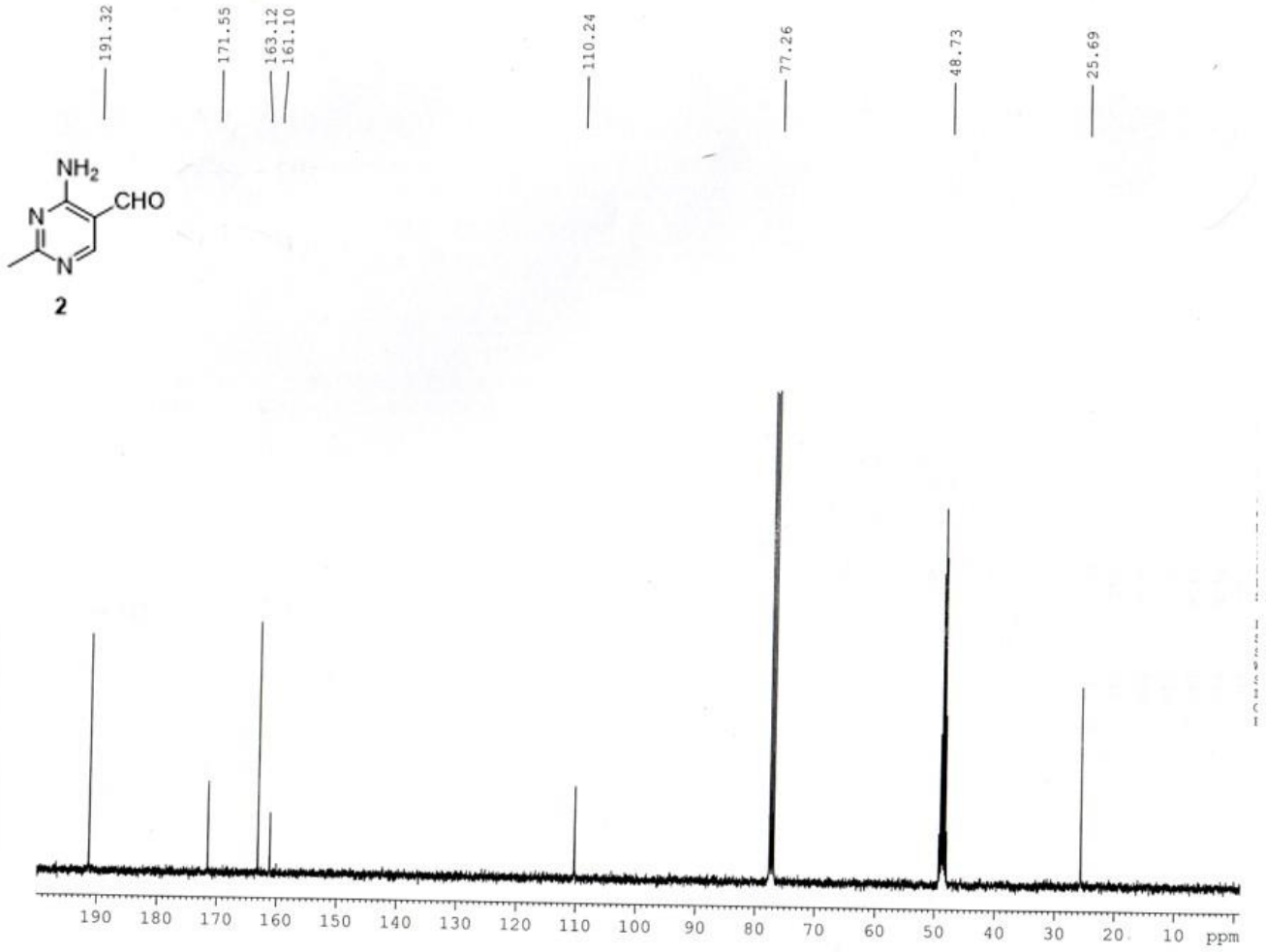
S2 – ^{13}C NMR spectrum of *4- Amino-2-methylpyrimidine- 5-carbonitrile (1)*



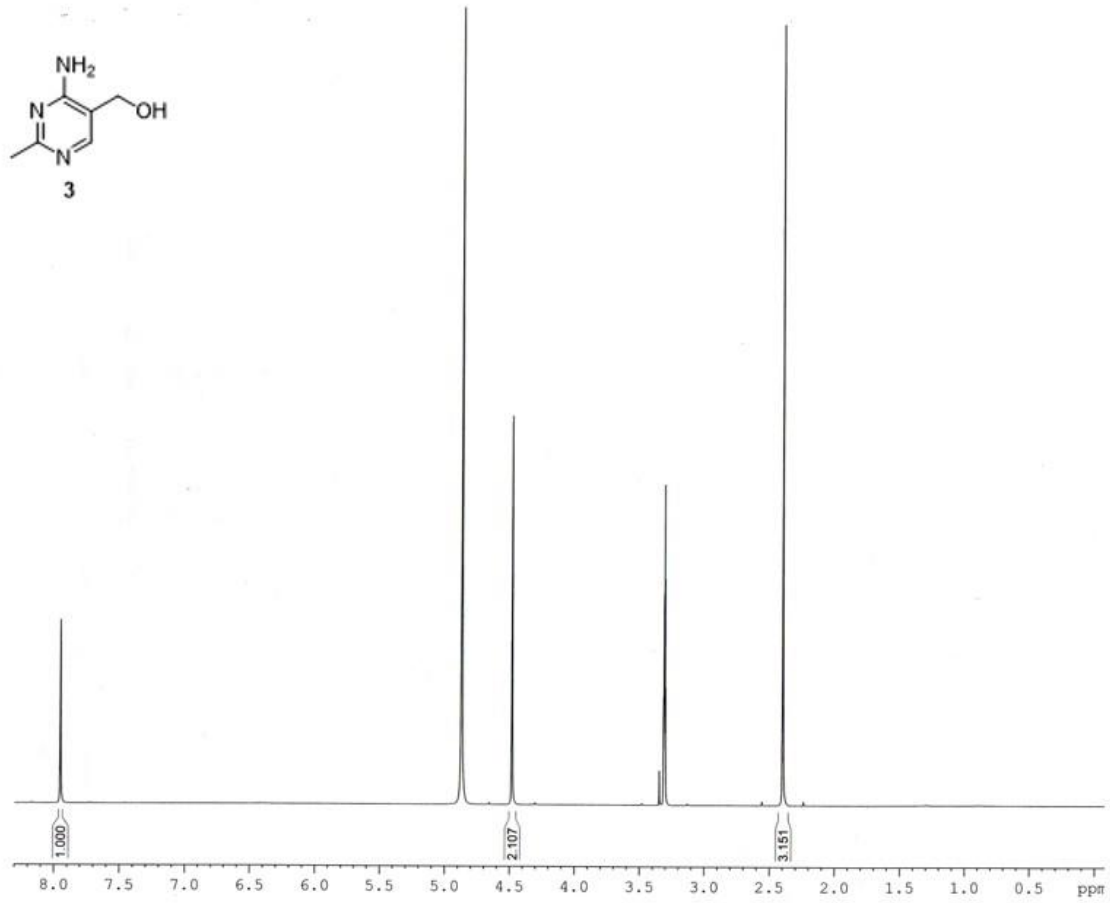
S3 – ^{1}H NMR spectrum of *4-Amino-2-methylpyrimidine-5-carboxaldehyde (2)*



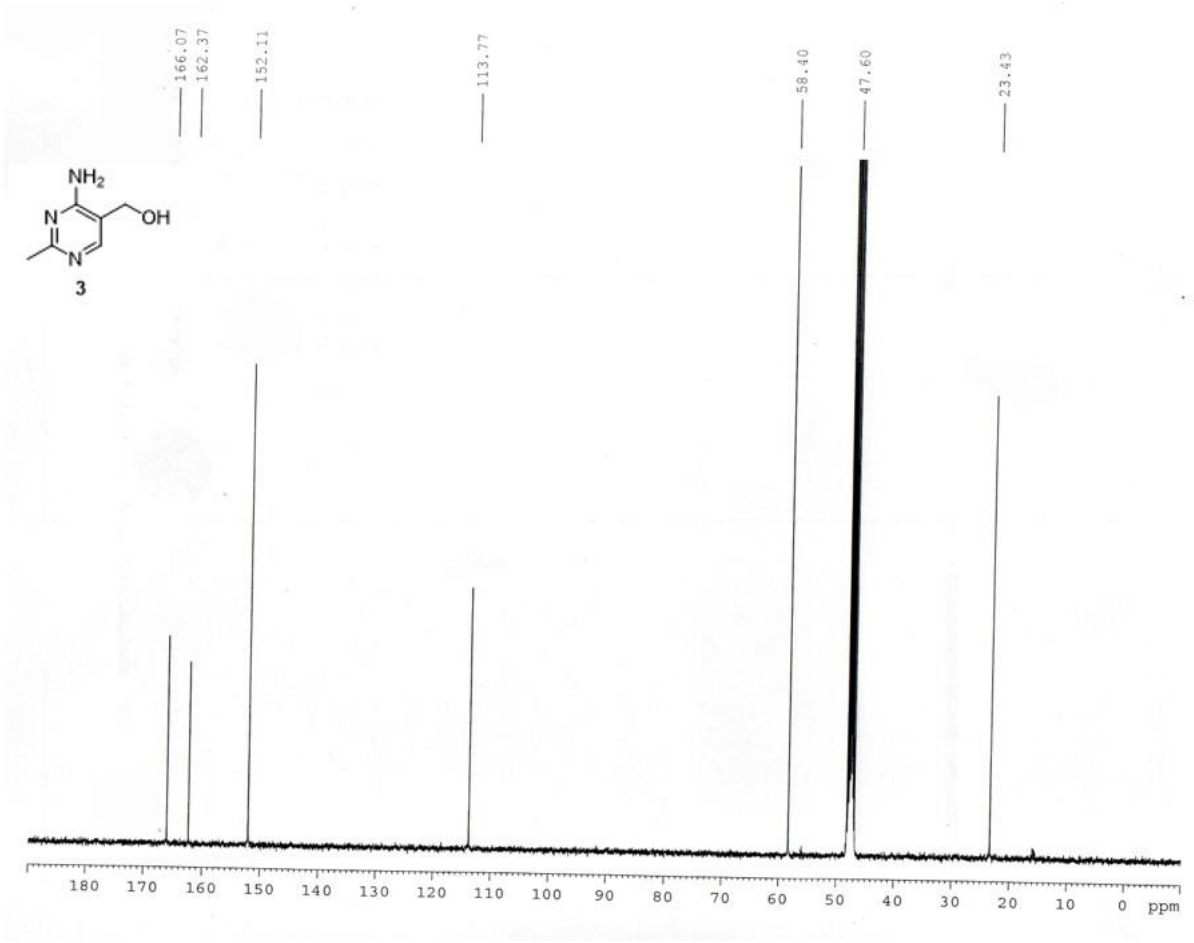
S4 – ^{13}C NMR spectrum of *4-Amino-2-methylpyrimidine-5-carboxaldehyde (2)*



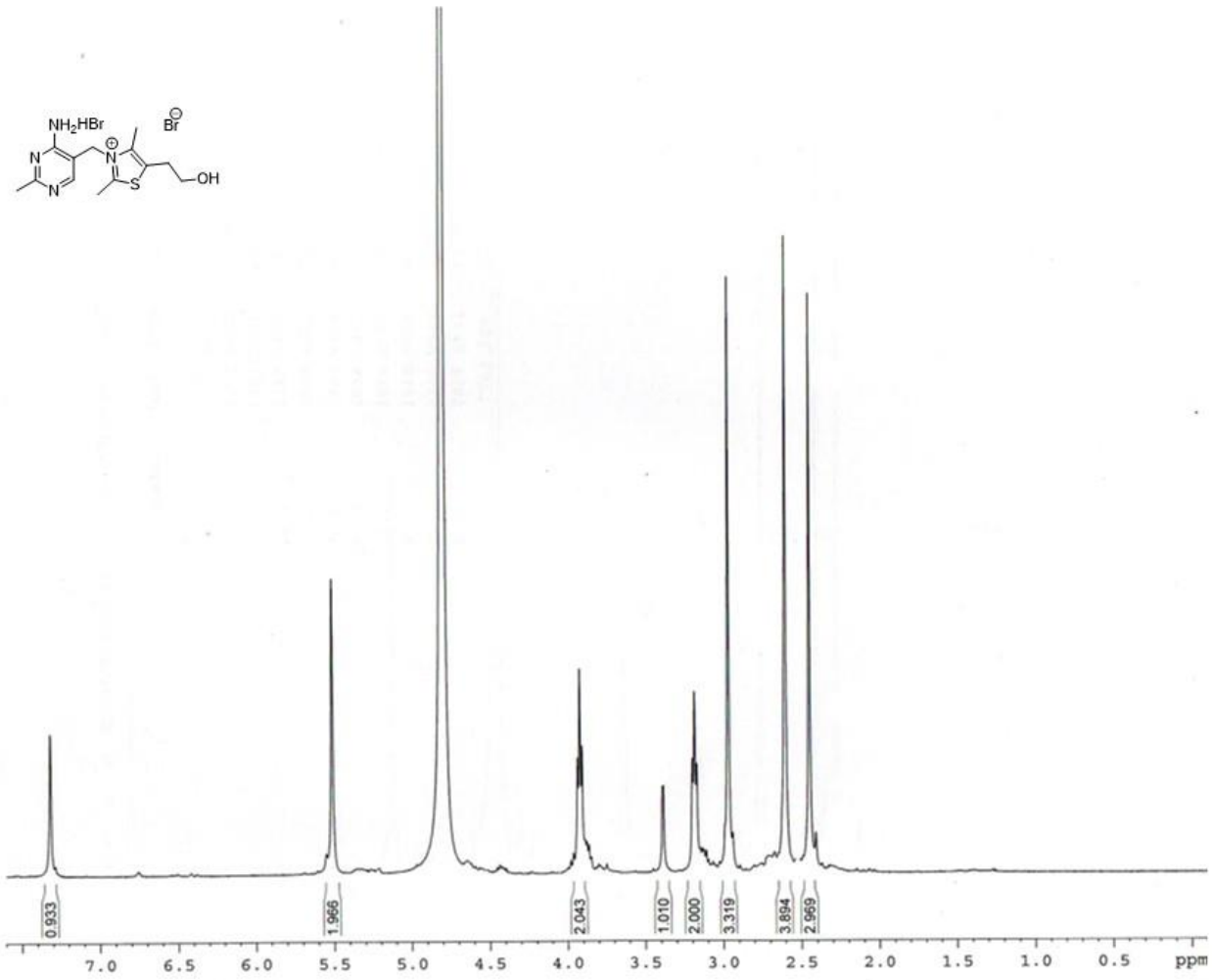
S5 – ^{1}H NMR spectrum of *(4-amino-2-methylpyrimidin-5-yl)methanol (3)*



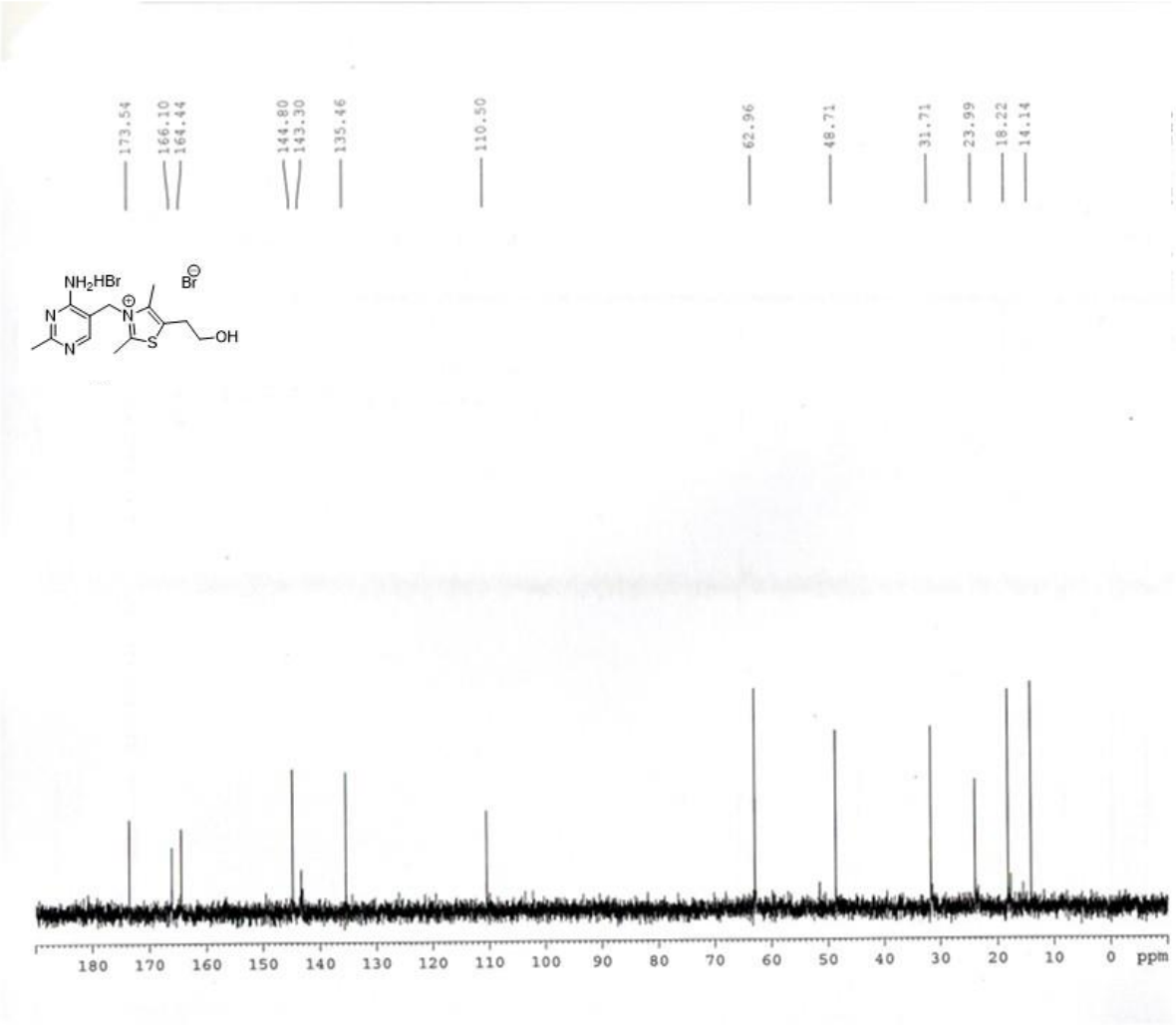
S6 – ^{13}C NMR spectrum of *(4-amino-2-methylpyrimidin-5-yl)methanol (3)*



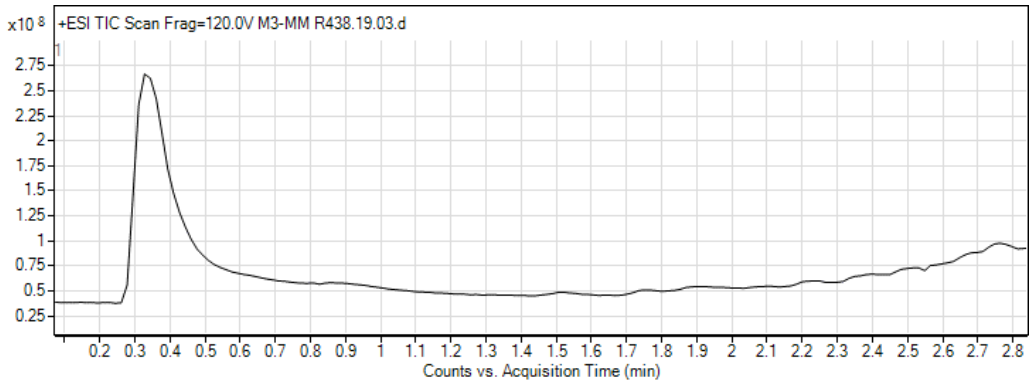
S7 – ^{1}H NMR spectrum of *2'-methylthiamine*



S8 – ^{13}C NMR spectrum of *2'-methylthiamine*



S9 – HPLC chromatogram of *2'-methylthiamine*



S10 – ESI-HRMS of *2'-methylthiamine*

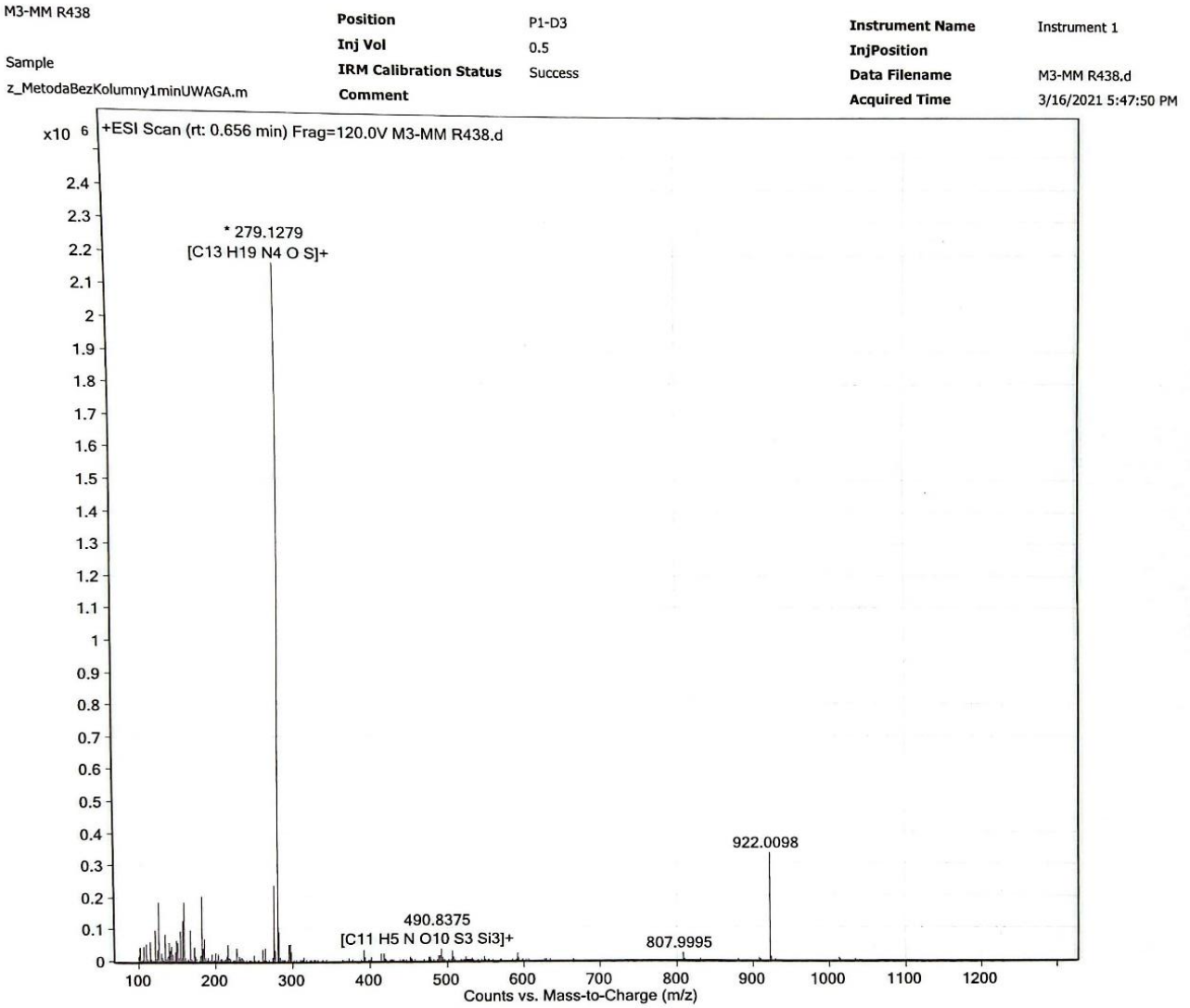


Table S1. Statistical parameters of 100-ns molecular dynamics simulation of OCT1 and its complexes. APO – unliganded form, TIA , MTA, OXT– complexes with thiamine, 2-methylthiamine and oxythiamine. Average - arithmetic mean, SD - standard deviation, SD/average - coefficient of variation.

RMSD

	APO	TIA	MTA	OXT
AVE	2.52	3.03	2.62	3.02
SD	0.36	0.37	0.48	0.67
SD/ave	0.14	0.12	0.18	0.22

SASA

	APO	TIA	MTA	OXT
AVE	26229.05	26148.81	26316.52	26072.81
SD	365.33	472.01	440.67	315.60
SD/ave	0.01	0.02	0.02	0.01

RG

	APO	TIA	MTA	OXT
AVE	27.89	27.61	27.94	27.45
SD	0.21	0.19	0.22	0.26
SD/ave	0.01	0.01	0.01	0.01

RMSF

	APO	TIA	MTA	OXT
AVE	1.45	1.44	1.25	1.51
SD	0.74	0.80	0.75	1.06
SD/ave	0.51	0.56	0.60	0.70