

Unexpected products of the reaction of purine nucleic base perchlorates with acetylacetone causing single-strand breaks in the DNA molecule

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Supplementary Information

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1. Quantum chemical calculations

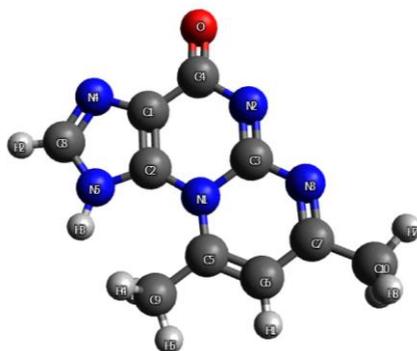


Figure S1 Model of 7,9-dimethylpyrimido[2,1-b]purin-4(1H)-one molecule

The charges were assessed using the Mulliken scheme.

Table 1 Partial charge on atoms of **4**

Atoms	Structure 4a	Structure 4b
C1	0.170	0.150
C2	0.150	0.140
C3	0.240	0.240
C4	0.300	0.30
C5	0.027	0.027
C6	-0.021	-0.021
C7	0.044	0.044
C8	0.096	0.096
C9	-0.024	-0.024
C10	-0.022	-0.022
N1	-0.270	-0.270
N2	-0.170	-0.170
N3	-0.220	-0.220
N4	-0.230	-0.220
N5	-0.330	-0.310
O	-0.260	-0.260

References

1. Paul V. Bernhardt, C. Wentrup, Structures of 4-Iminopyrido[1,2-a]pyrimidines, Pyrido[1,2-a]pyrimidin-4-ones, Pyridopyrimidinium Olates, and Thiazolo[3,2-a]pyrimidine Analogues, *Aust. J. Chem.* 2012, 65, 371–375.
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2. NMR spectra of synthesized compounds

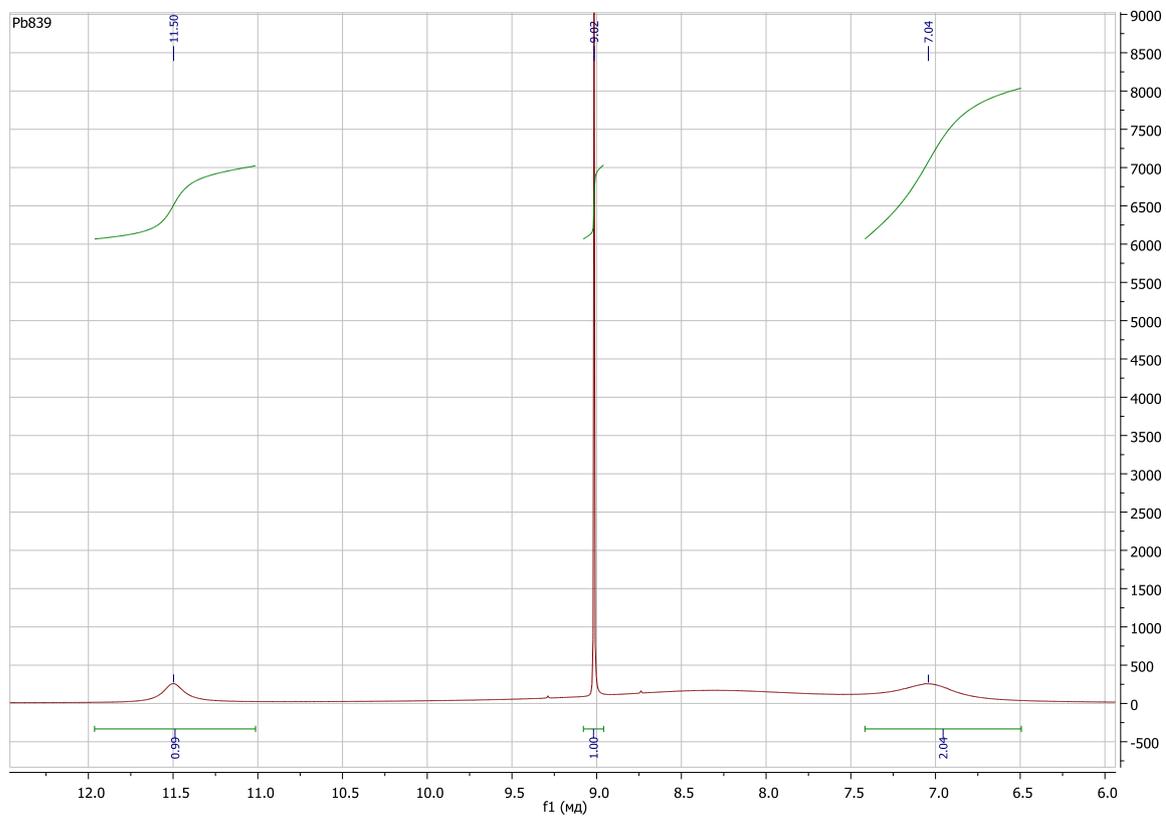
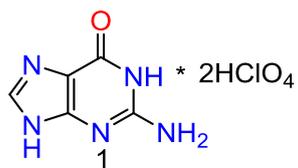


Figure S2.1 ¹H NMR spectra for guanine dicationic salt

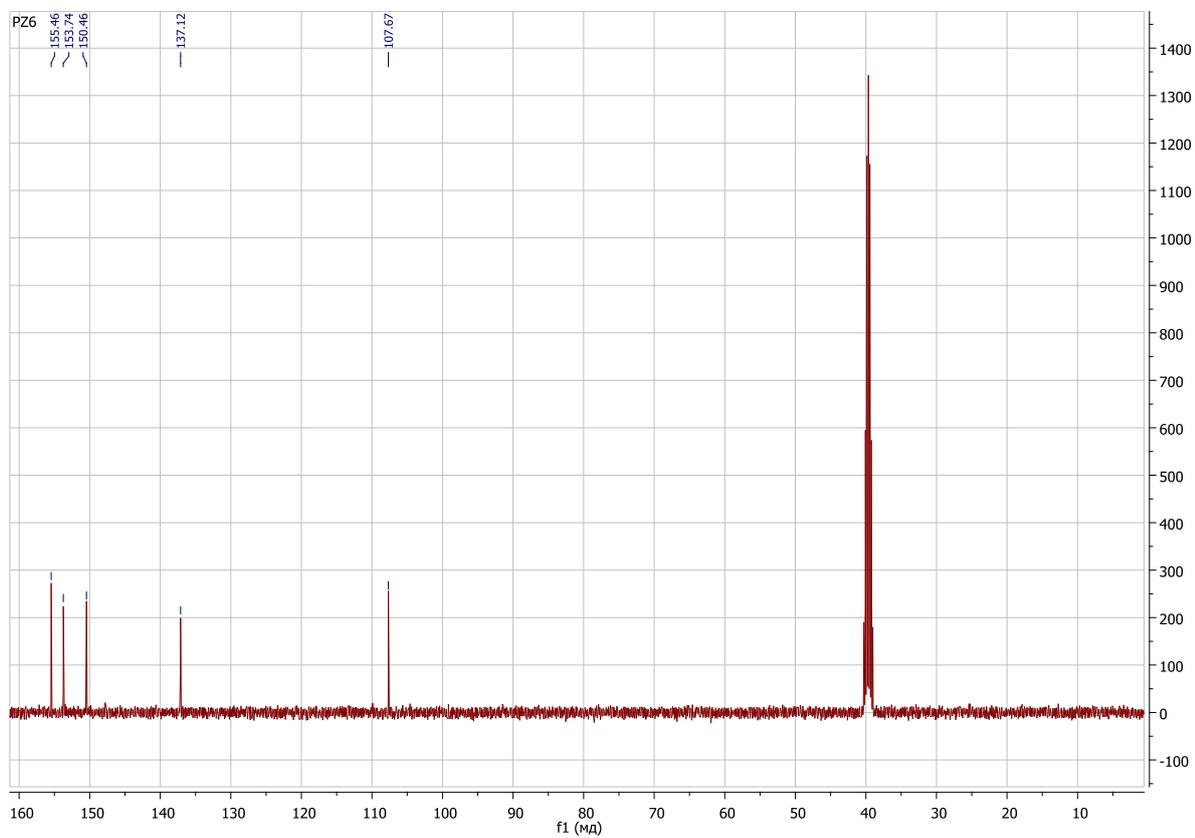
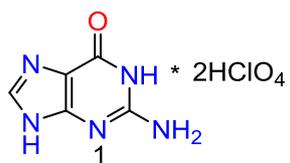


Figure S3.2 ¹³C NMR spectra for guanine dication perchlorate

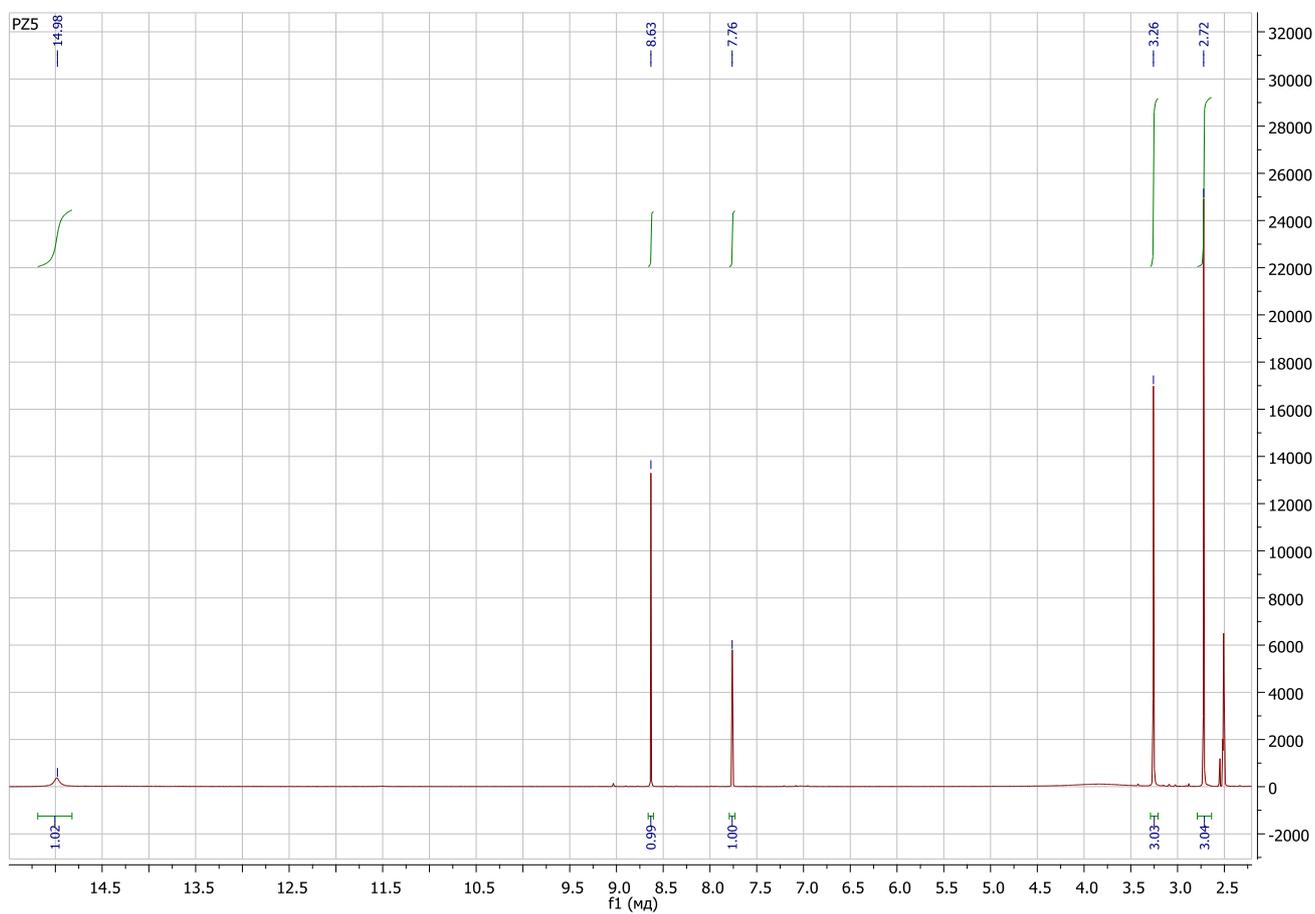
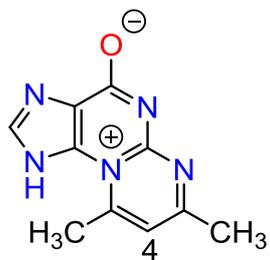


Figure S2.3 ¹H NMR spectra for 7,9-dimethylpyrimido[2,1-b]purin-4(1H)-one

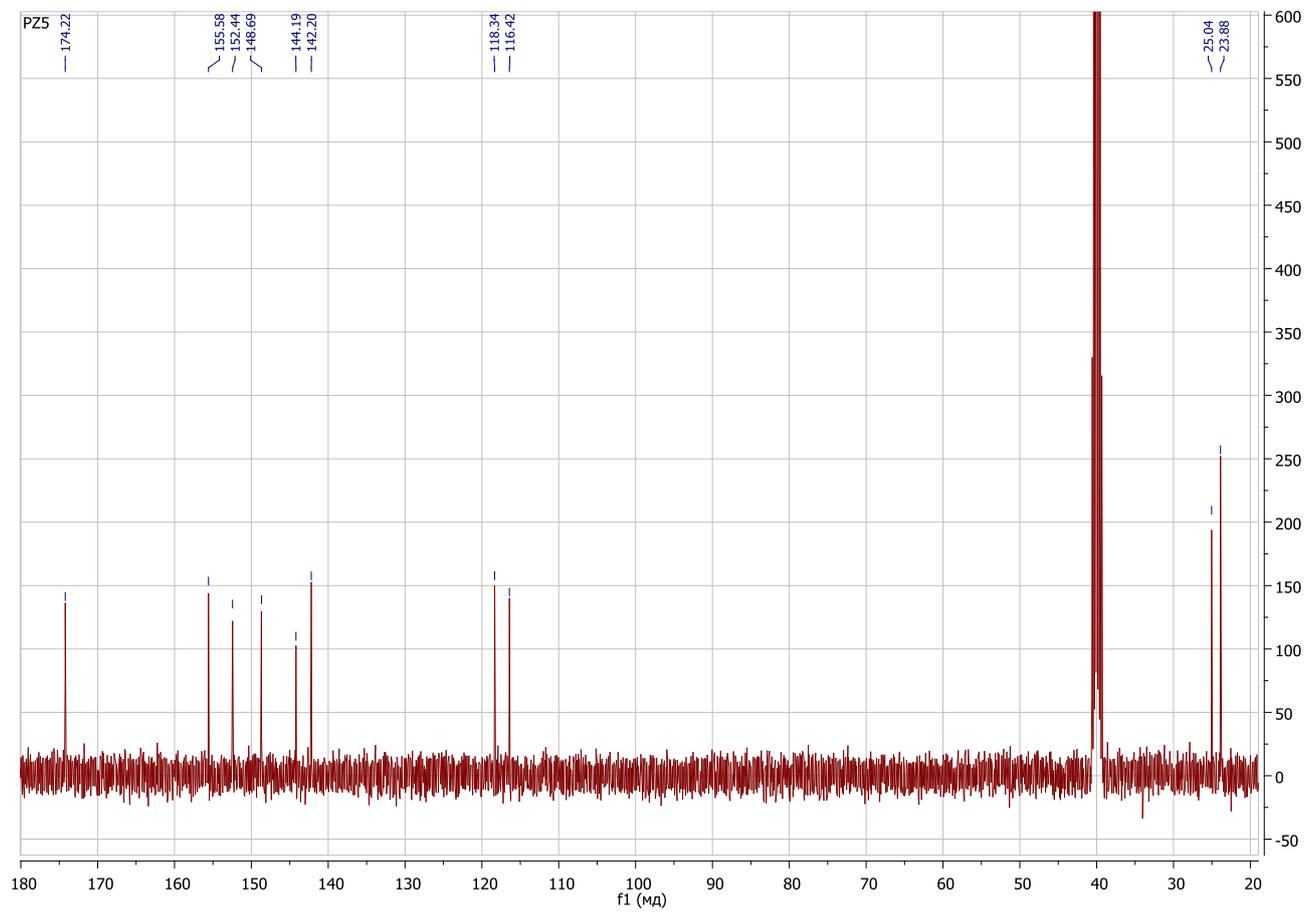
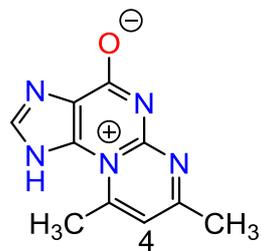


Figure S2.4 ¹³C NMR spectra for 7,9-dimethylpyrimido[2,1-b]purin-4(1H)-one

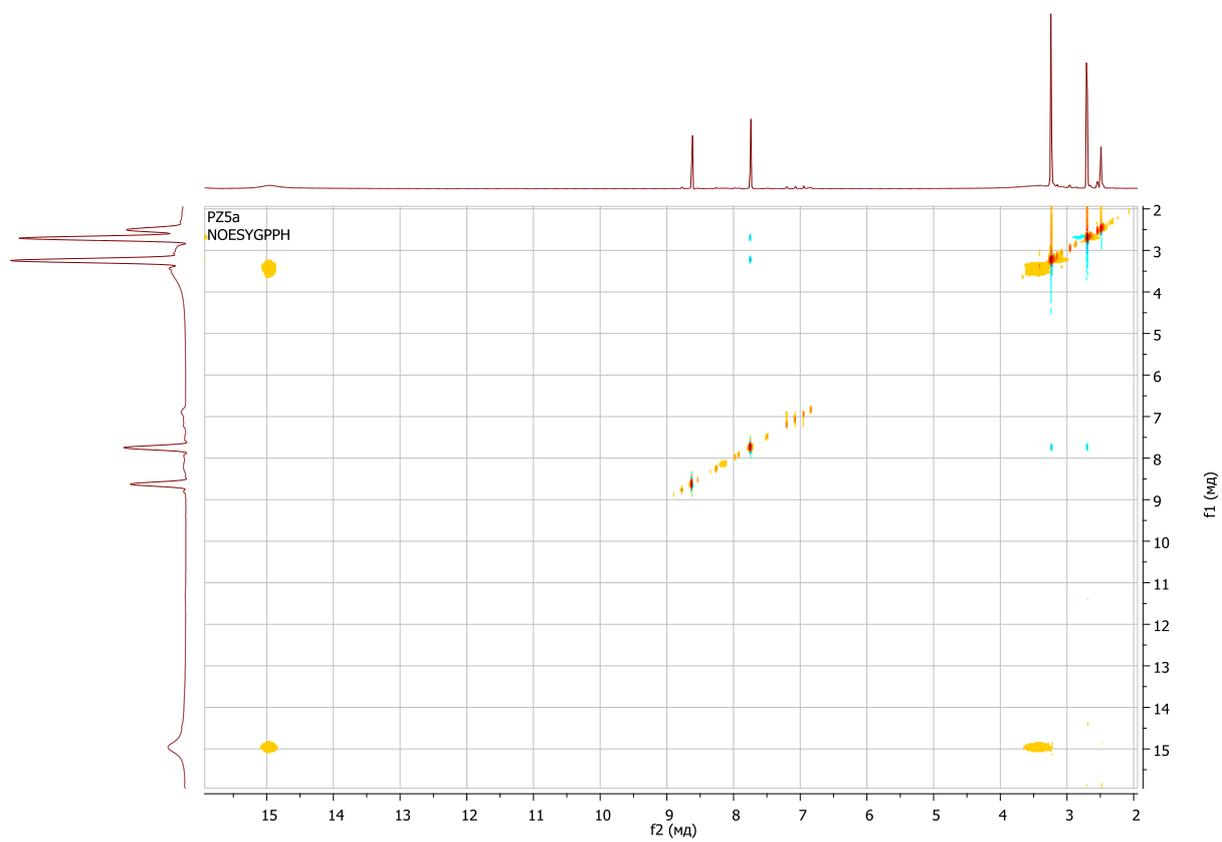
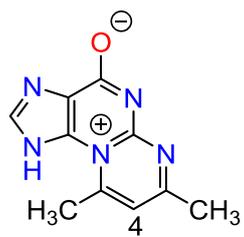


Figure S2.5 NOESY NMR spectra for 7,9-dimethylpyrimido[2,1-*b*]purin-4(1H)-one

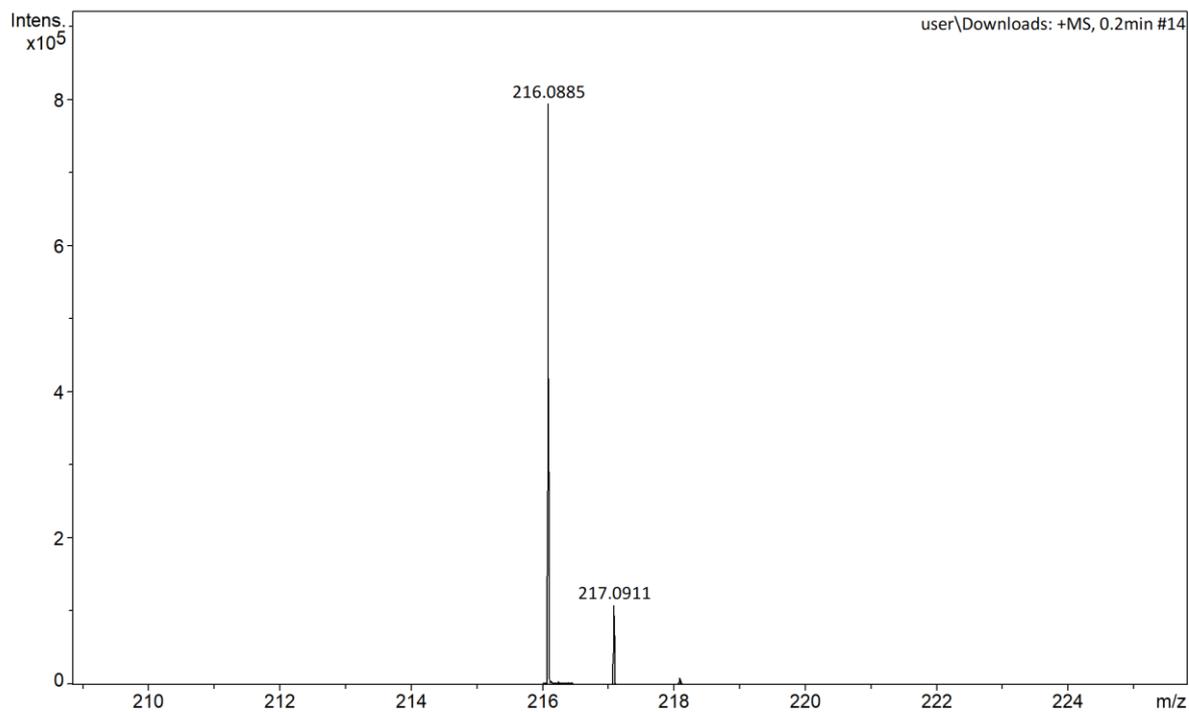
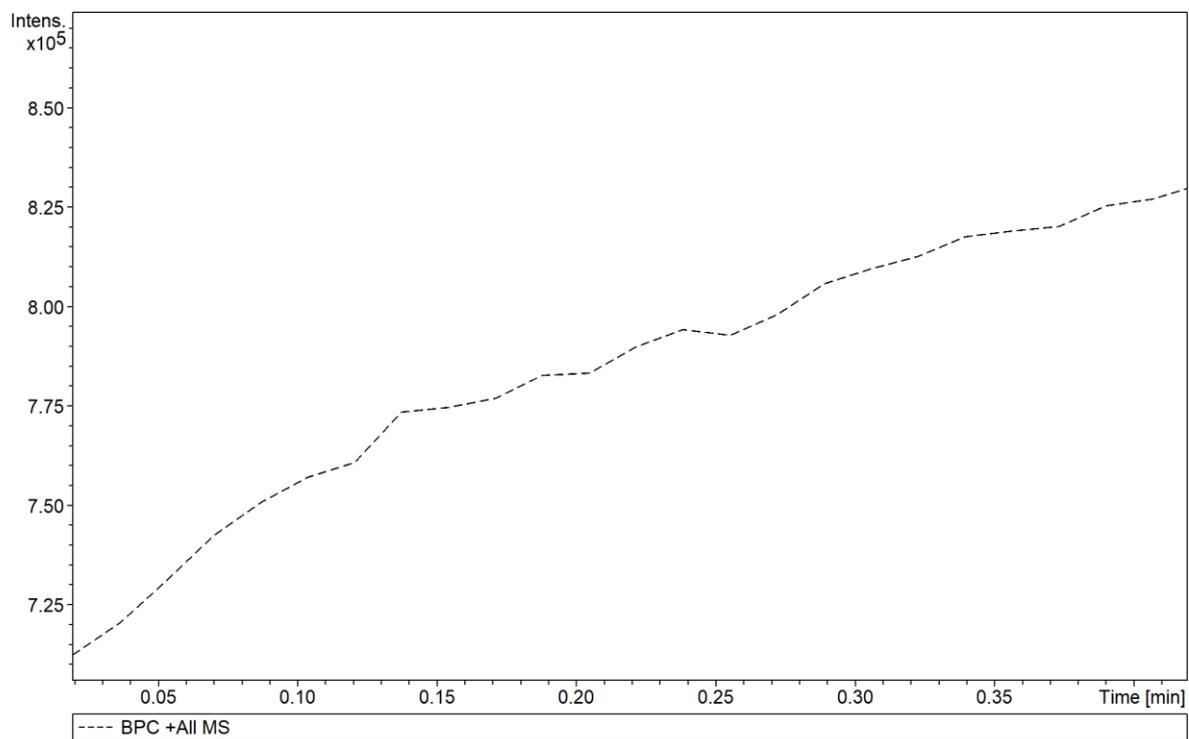
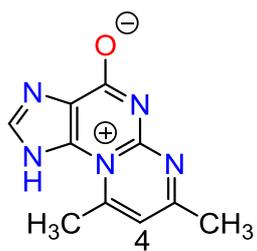


Figure S2.6 Mass spectrum for 7,9-dimethylpyrimido[2,1-b]purin-4(1H)-one

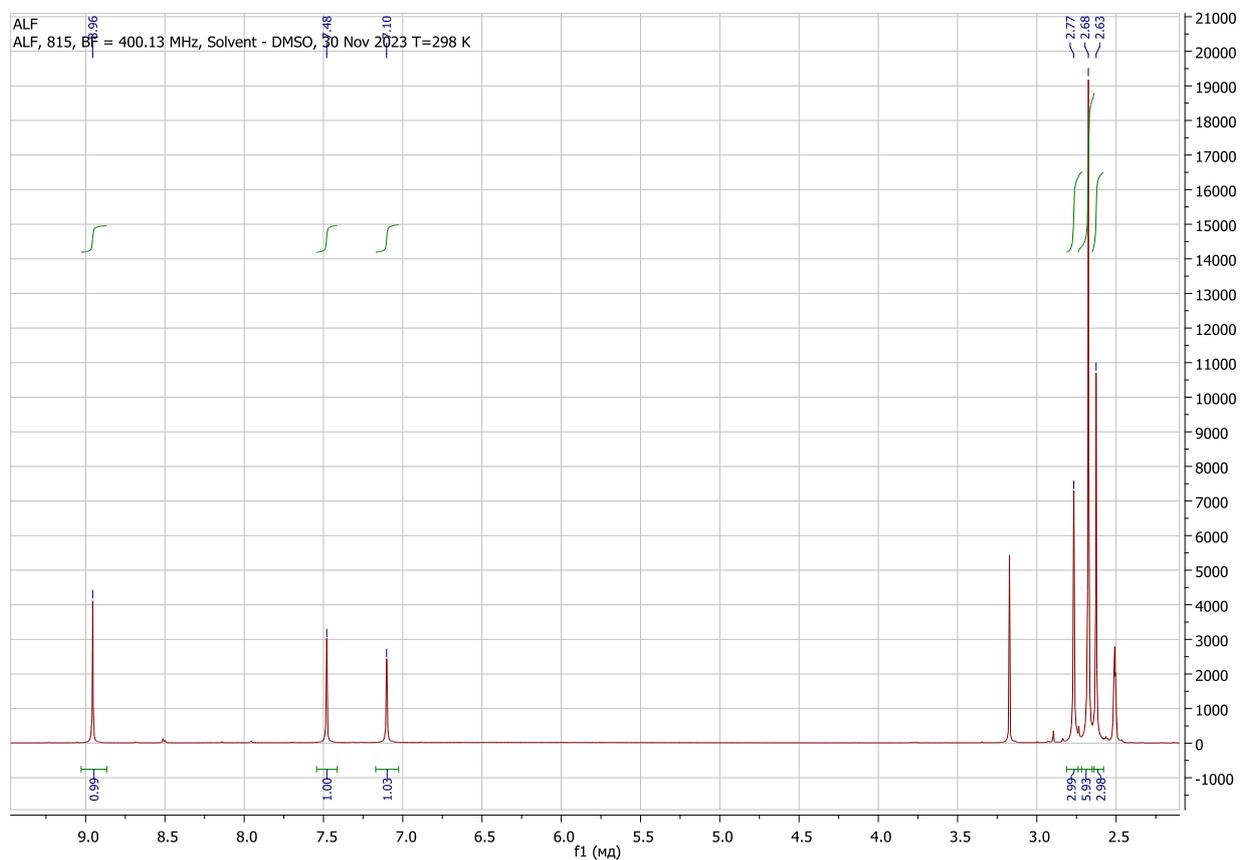
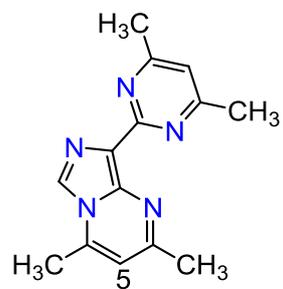


Figure S2.7 ^1H NMR spectra for 8-(4,6-dimethylpyrimidin-2-yl)-2,4-dimethylimidazo[1,5-a]pyrimidine

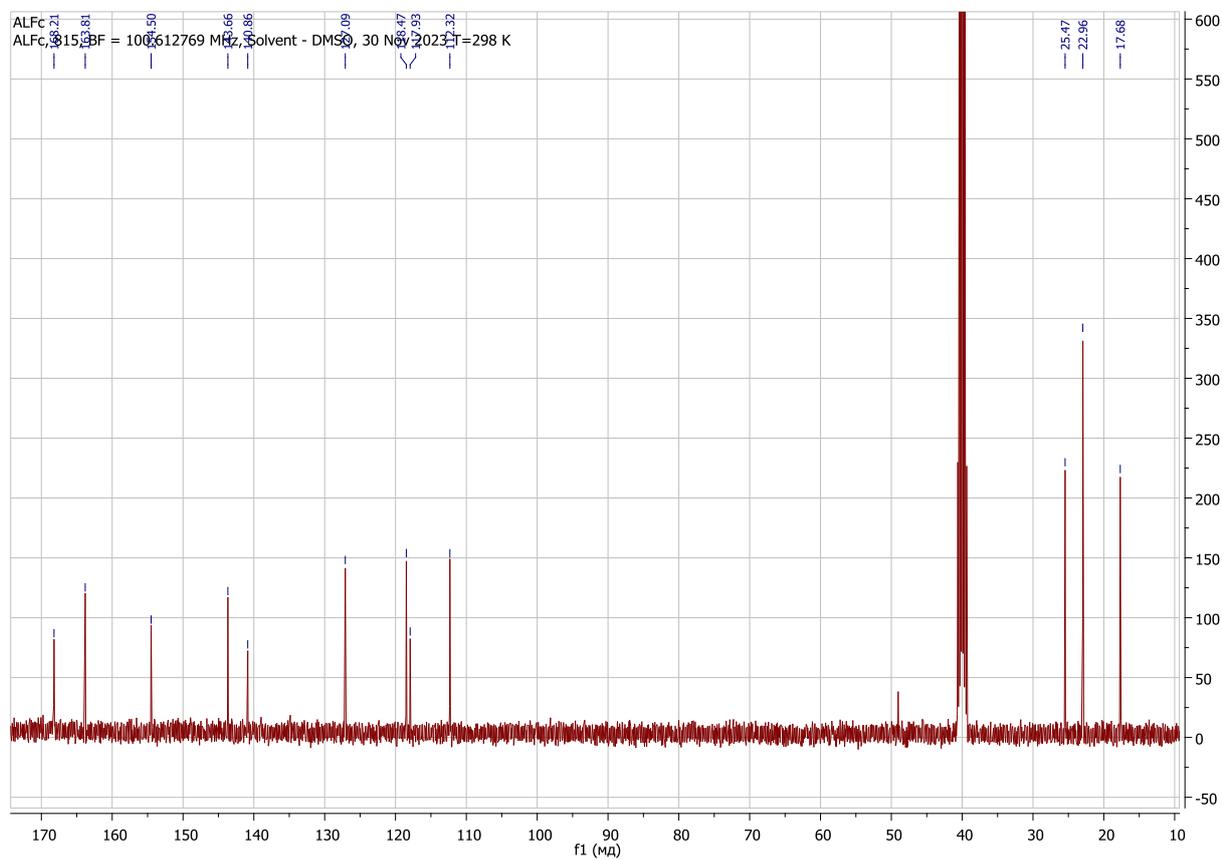
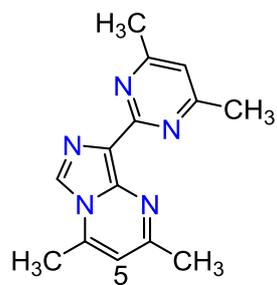


Figure S2.8 ^{13}C NMR spectra for 8-(4,6-dimethylpyrimidin-2-yl)-2,4-dimethylimidazo[1,5-a]pyrimidine

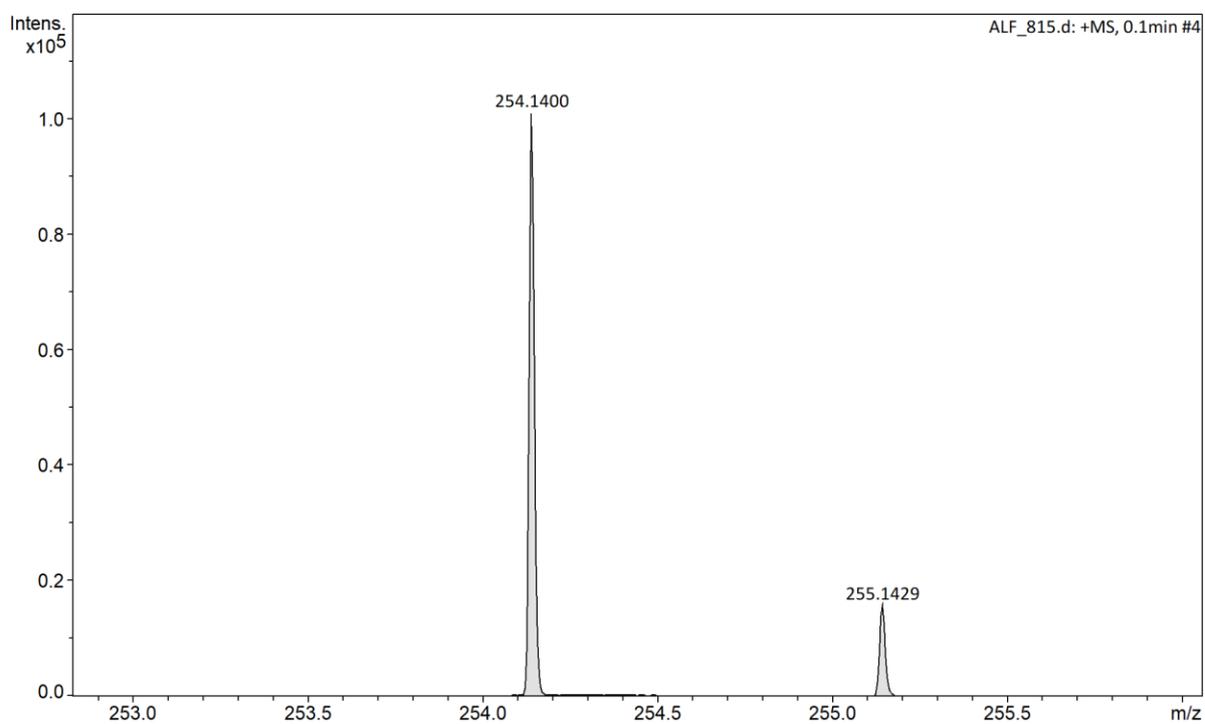
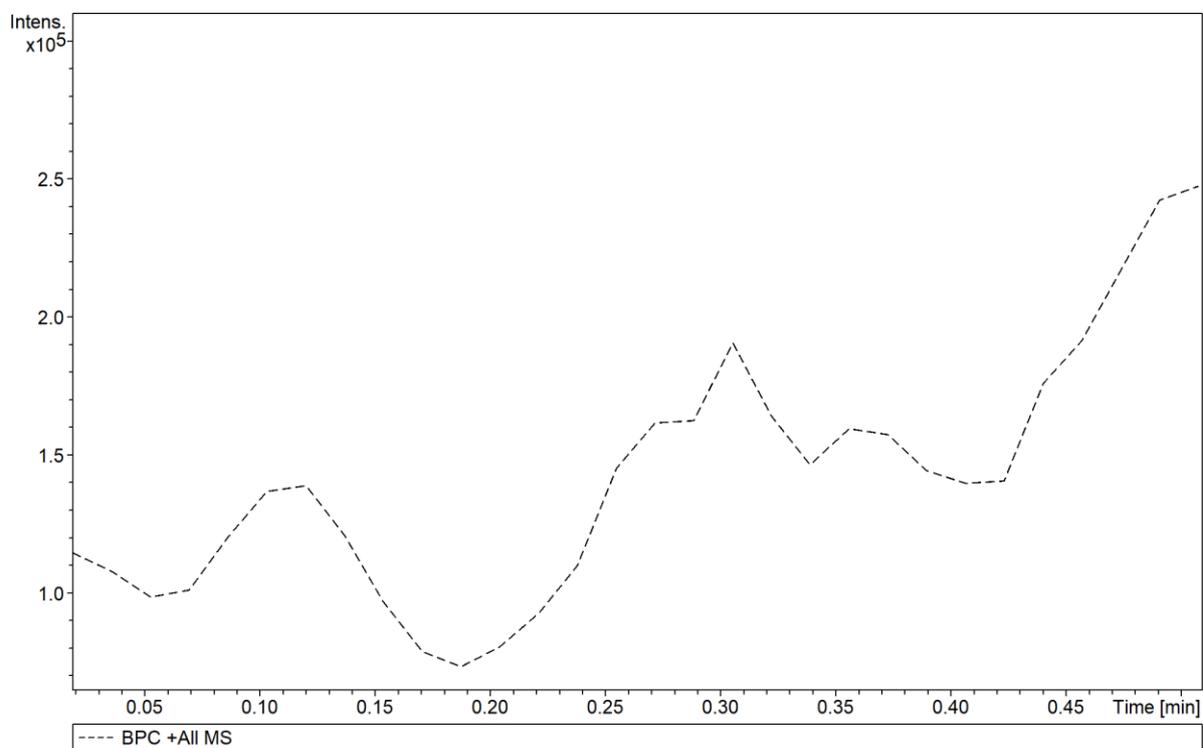
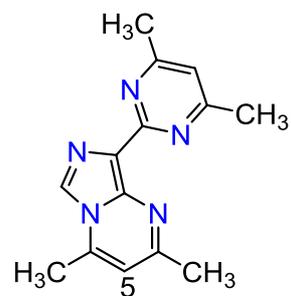


Figure S2.9 Mass spectrum for 8-(4,6-dimethylpyrimidin-2-yl)-2,4-dimethylimidazo[1,5-a]pyrimidine

3. Raw pictures of the electropherogram for 4 and 5

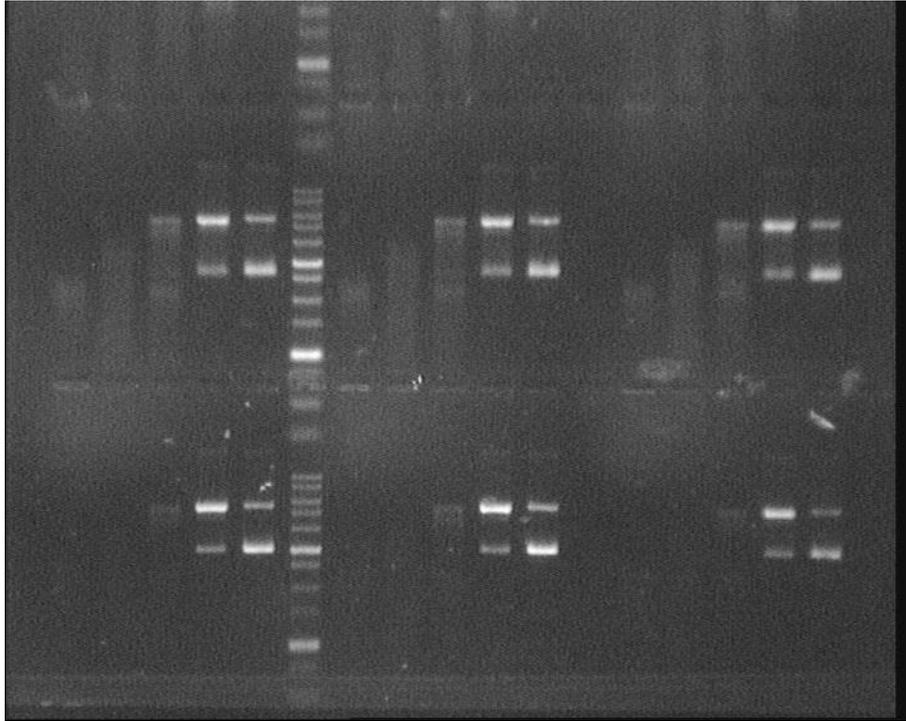


Figure S3.1. Raw picture of the electropherogram, demonstrating the results of pBR322 plasmid incubation in the presence of different concentrations of substance 4 (5-0,625 mM). Experiments were done in triplicate (three series from left to right). Two aliquots of each probe were analysed by electrophoresis (1 – upper part of the gel, 2 – lower part).

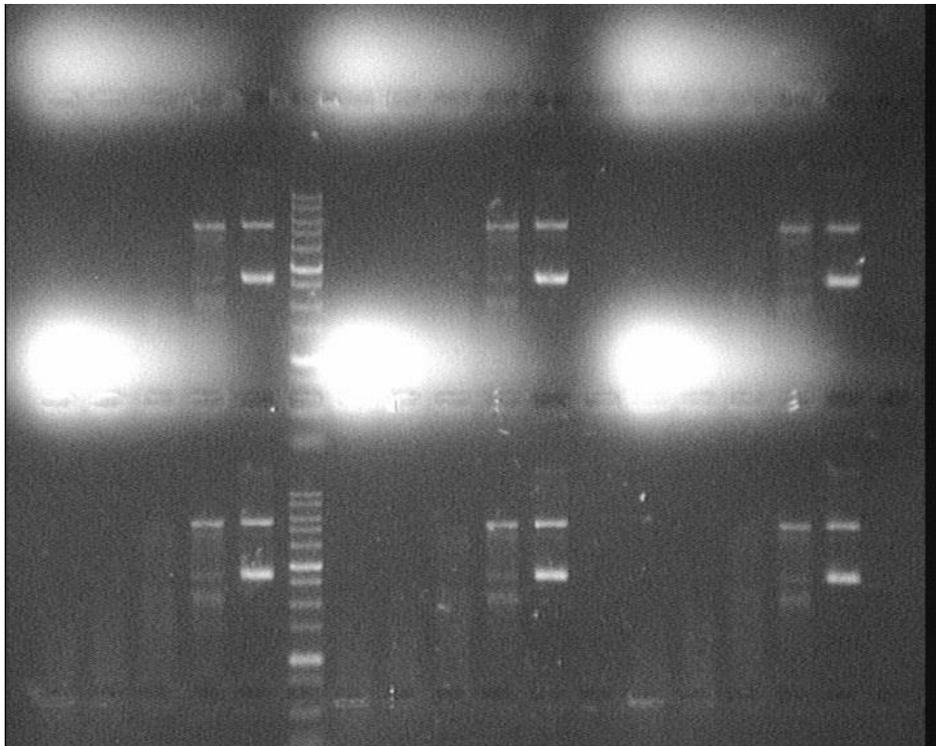


Figure S3.2. Raw picture of the electropherogram, demonstrating the results of pBR322 plasmid incubation in the presence of different concentrations of substance 5 (5-0,625 mM). Experiments were done in triplicate (three series from left to right). Two aliquots of each probe were analysed by electrophoresis (1 – upper part of the gel, 2 – lower part).