

Supporting Information

Synthesis and DNA polymerase recognition of 2'-deoxyribonucleoside triphosphates bearing 4-phenyl and 4-pyrimidinyl imidazoles as nucleobases

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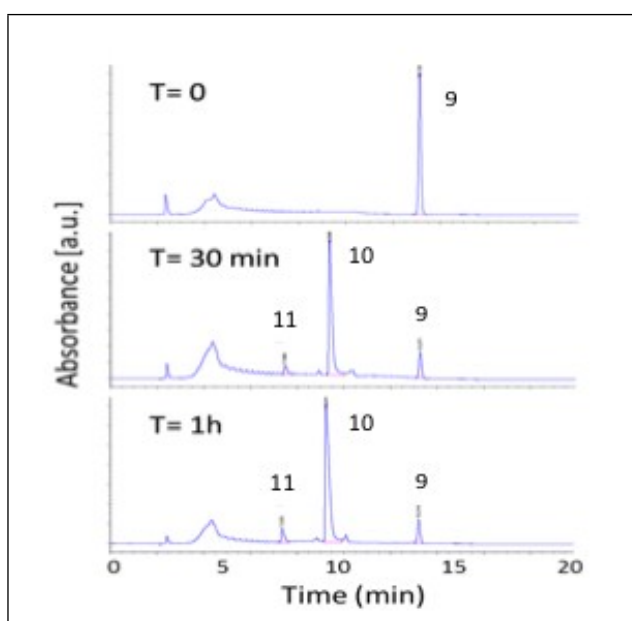
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Table S1. % Conversion of **9** into phosphorylated products **10** and **11** as a function of temperature/time

Temperature	POCl ₃ (equiv)	after 30 min			after 60 min		
		% 9	% 10	% 11	% 9	% 10	% 11
2°C (ice bath)	1.20	1	65	34	ND	ND	ND
-5°C	1.15	ND	ND	ND	0	78	22
-5°C	1.05	12	82	6	9	84	7
-10°C	1.15	1	86	12	0	82	18
-10°C	1.05	15	80	5	8	85	7

Reaction conditions: (**9**) (0.1 mmol) and proton sponge (1.2 equiv) in PO(OMe)₃ (0.9 mL) was stirred for 10 min at the indicated temperature, then POCl₃ (as indicated) in PO(OMe)₃ (0.1 mL) was added dropwise. Aliquots of the reaction mixture were hydrolysed after 30 and 60 min and analysed by HPLC (detection at 230 nm).

Figure S1. HPLC monitoring at 230 nm of phosphorylation reaction



Reaction conditions: 1.05 equiv POCl₃ at -5°C (Table S1); Analytical C18 column, 0-20% linear gradient of acetonitrile in 40 mM TEAA buffer over 20 min. Retention times (t_R): 7.37 min for **11**, 9.24 min for **10**, 13.20 min for **9**.

Oligodeoxynucleotide sequences used in PEX experiments

Name	Sequence
P1	5'-ATTGGTAGCACGGTCAGTTCGGAGT-3'
T5	3'-TAACCATCGTGCCAGTCAAGCCTCAAAAAA-5'
P3	5'-CAGGAAACAGCTATGAC-3'
T6	3'-GTCCTTTGTCGATACTGTTTTT-5'

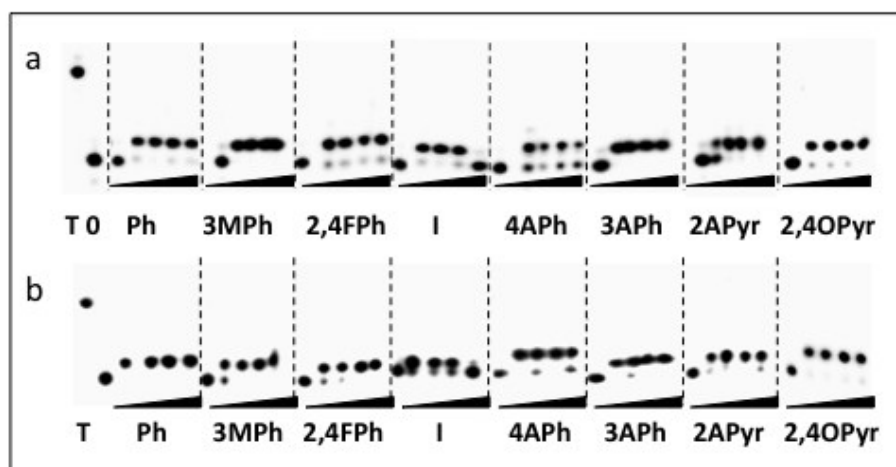


Figure S2. PAGE analysis of primer extension experiments with KF (exo-) using template T5 after incorporation of an analogue (0, 10, 25, 100, 250 μM as indicated by the arrow) or dTTP (10 μM) in the absence or presence of Mn^{2+} ions (0.25 mM) (Panel a or b, respectively).

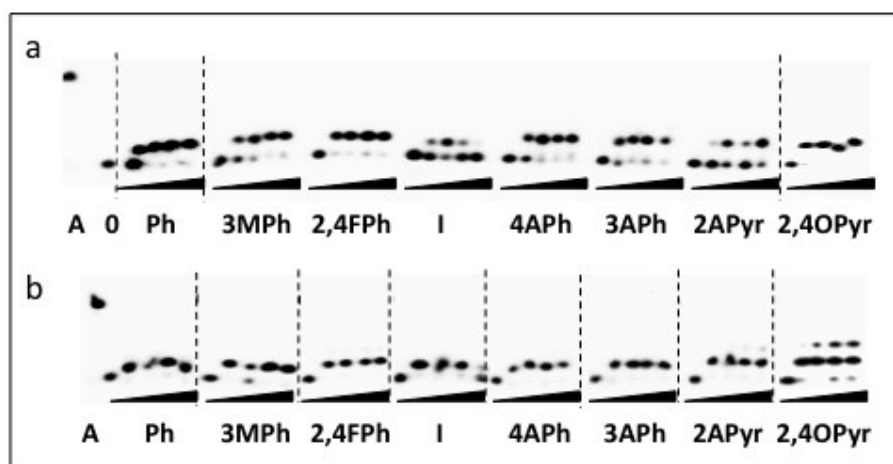


Figure S3. PAGE analysis of primer extension experiments with KF (exo-) using template T6 after incorporation of an analogue (0, 10, 25, 100, 250 μM μM as indicated by the arrow) or dATP (10 μM) in the absence or presence of Mn^+ ions (0.25 mM) (Panel a or b, respectively).

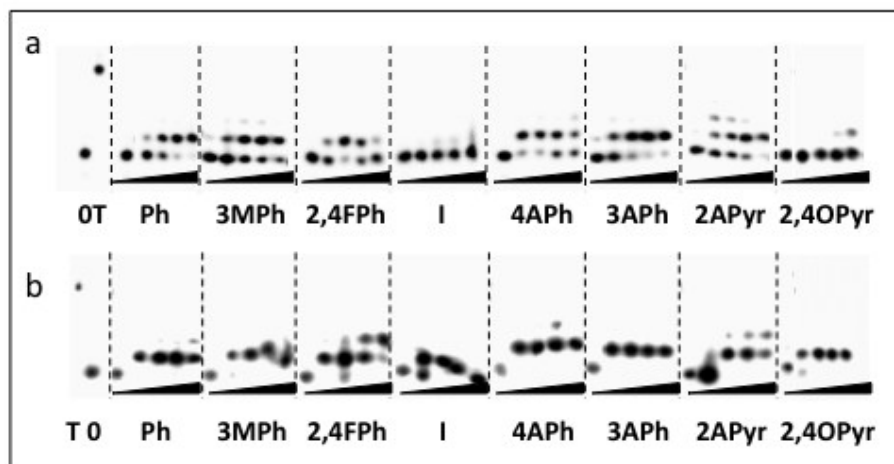
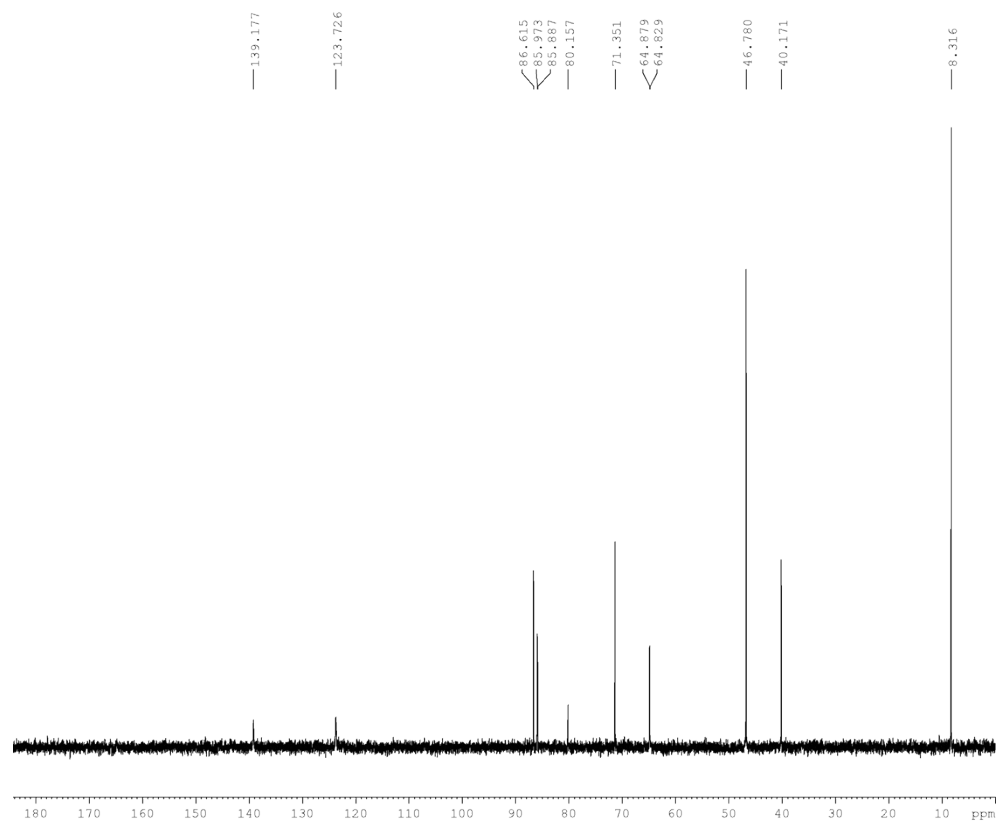
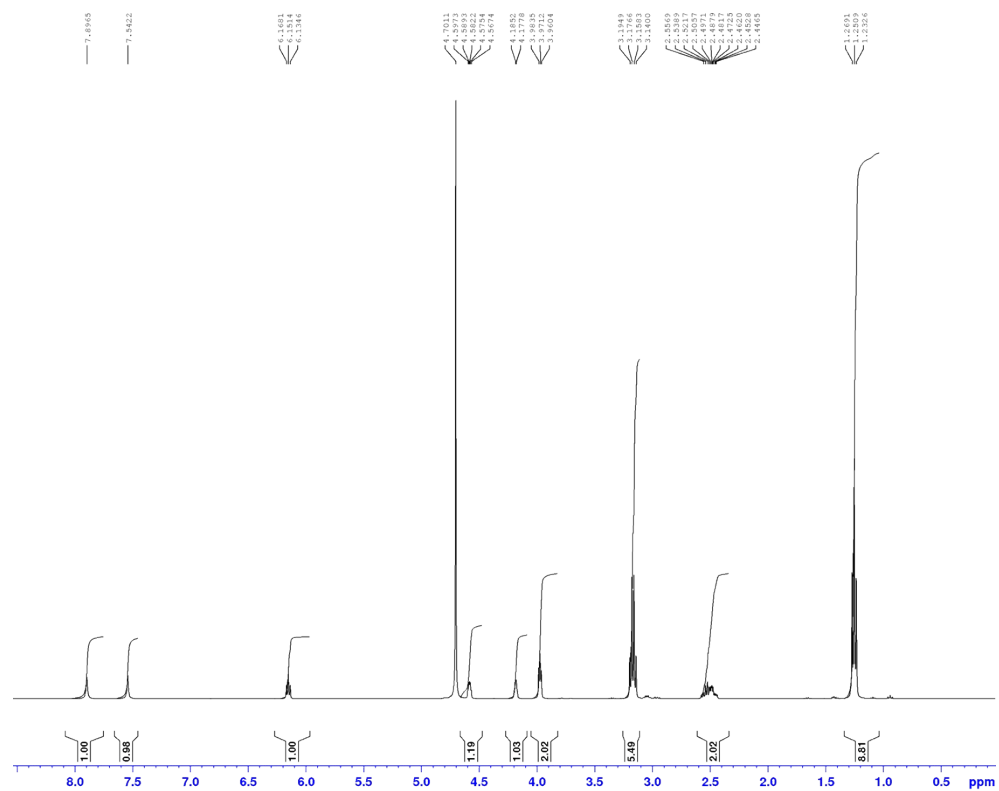
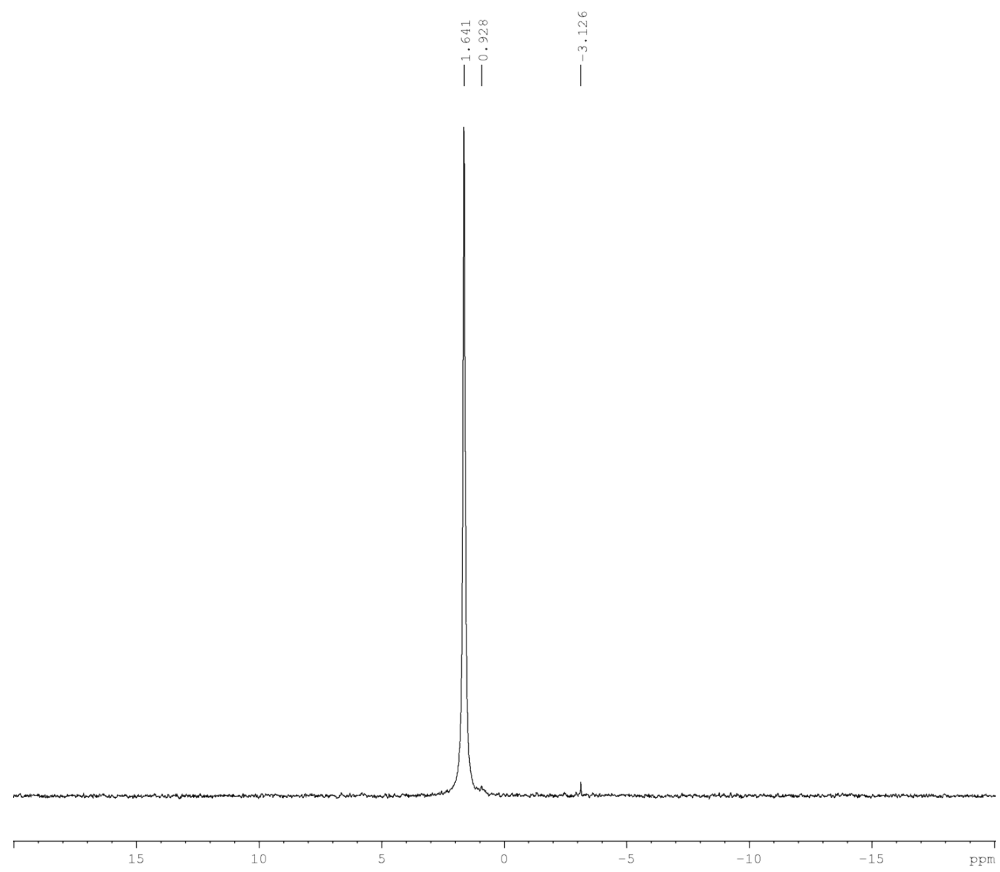


Figure S4. PAGE analysis of primer extension experiments with Vent (exo-) using template T5 after incorporation of an analogue (0, 10, 25, 100, 250 μM μM as indicated by the arrow) or dTTP (10 μM , noted T)

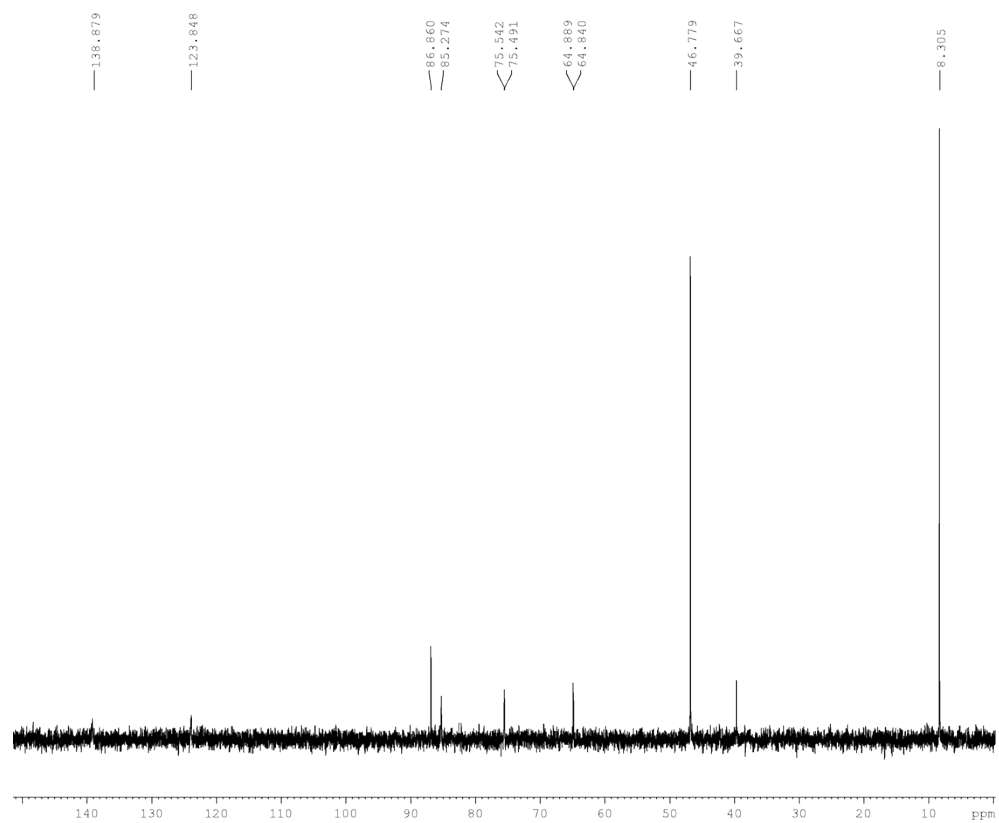
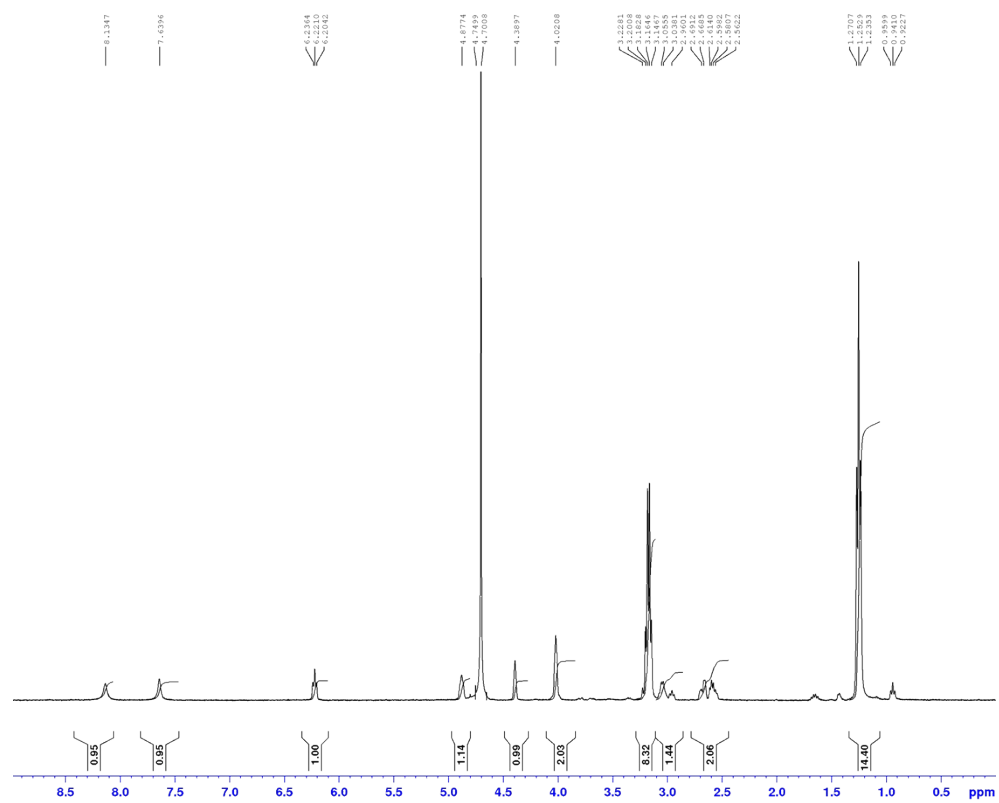
in the absence or presence of Mn^{2+} ions (0.25 mM) (Panel a or b, respectively).

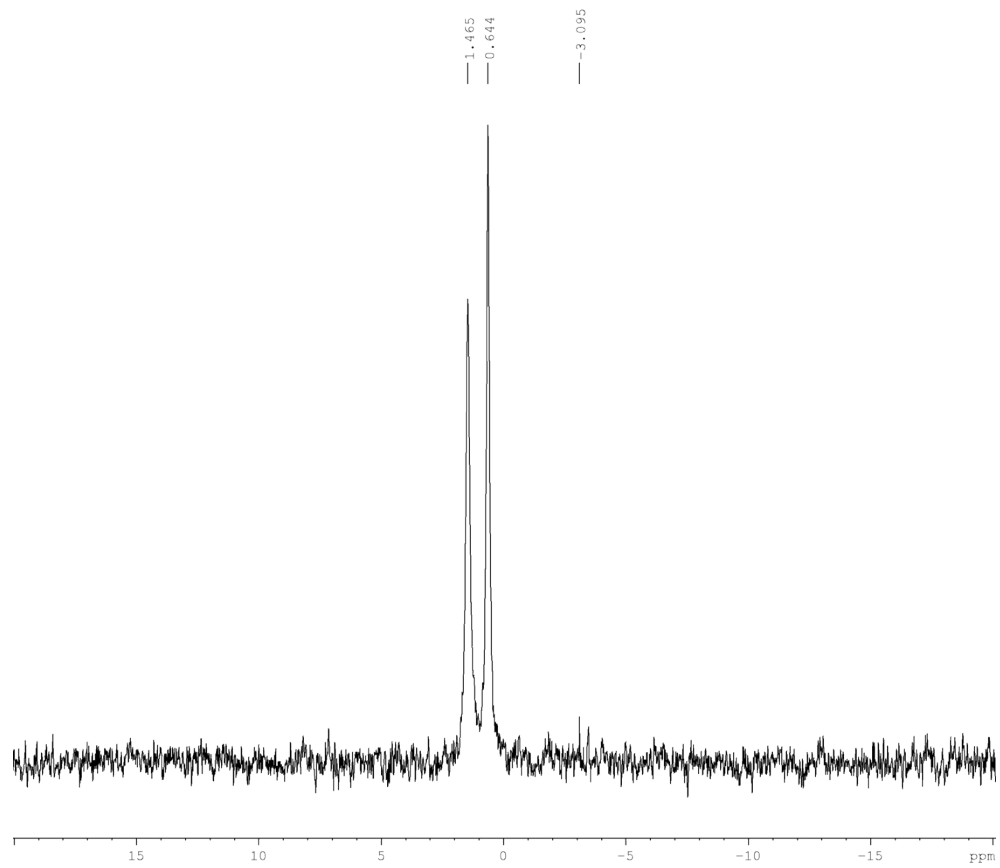
1-(2-Deoxy-β-D-ribofuranosyl)-4-iodo-1*H*-imidazole-5'-*O*-monophosphate (10)



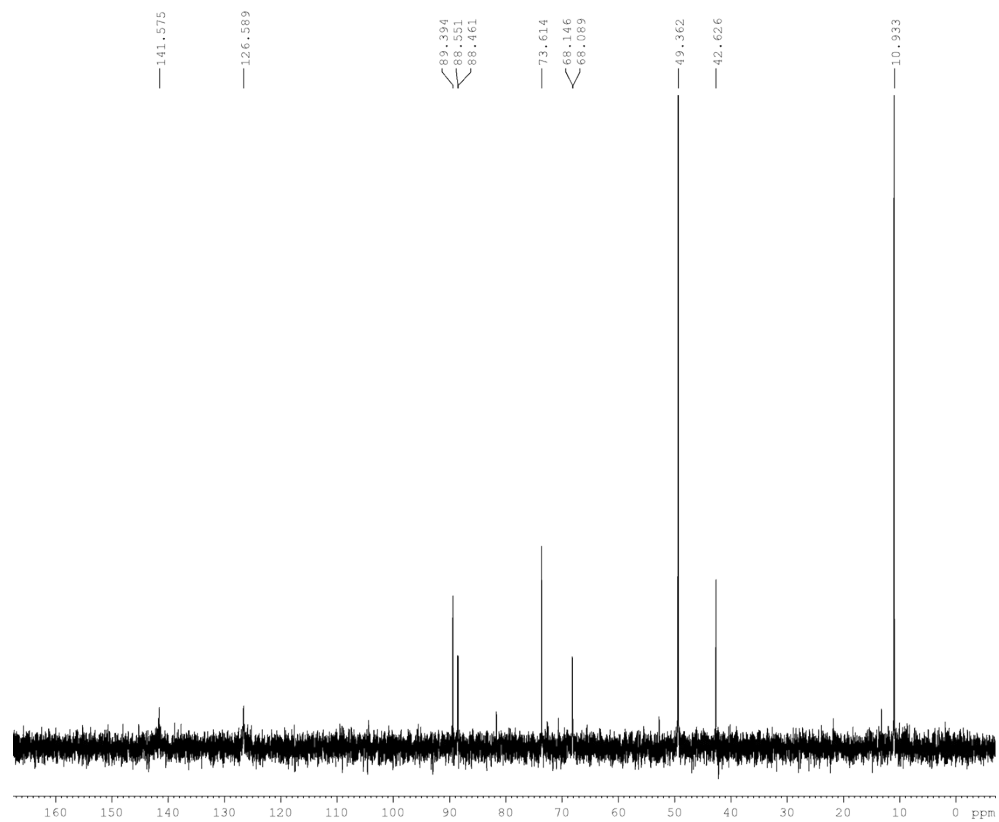
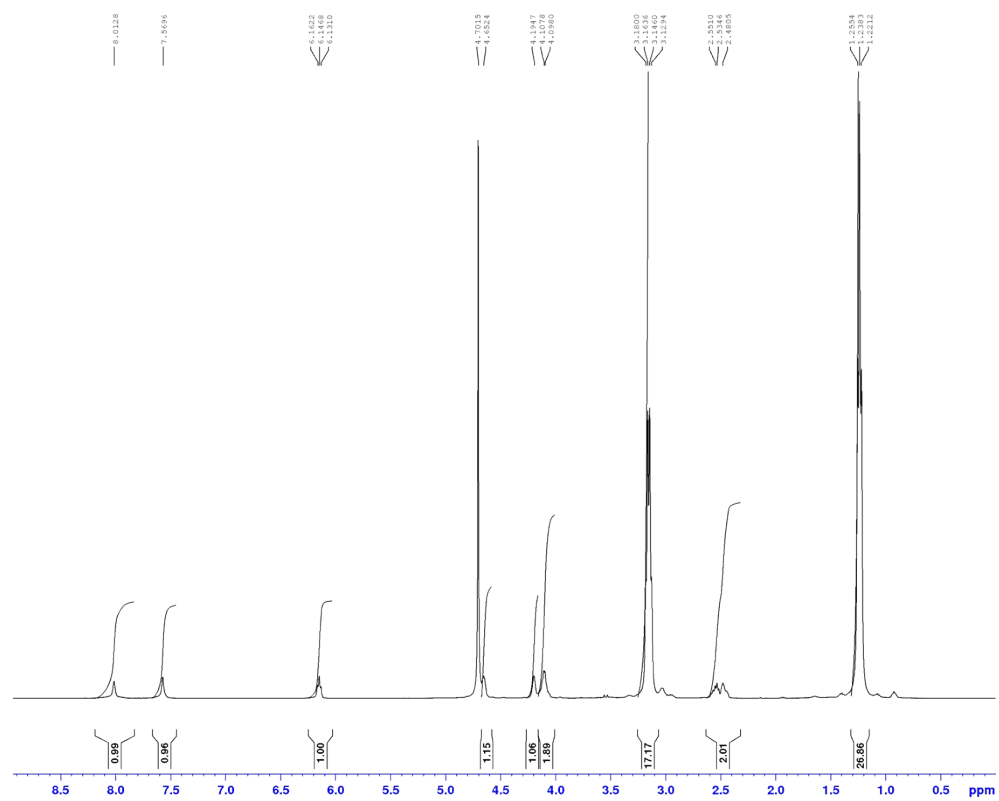


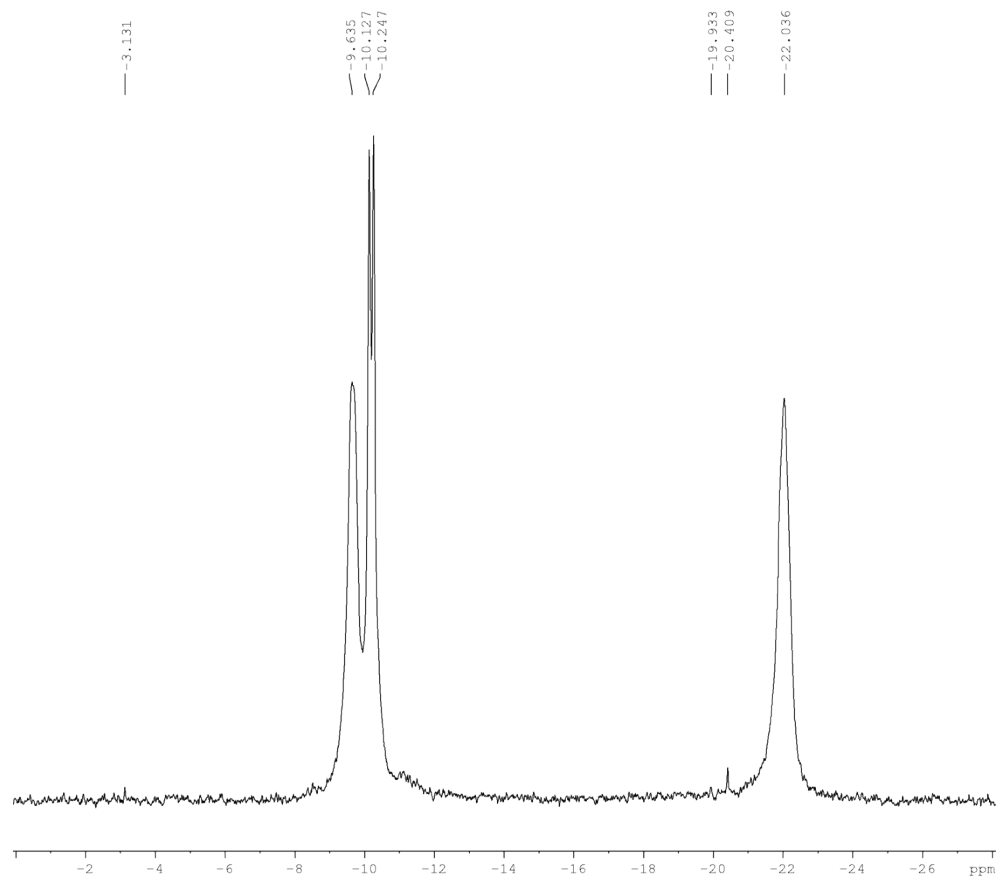
1-(2-Deoxy-β-D-ribofuranosyl)-4-iodo-1H-imidazole-3', 5'-O-diphosphate (11)



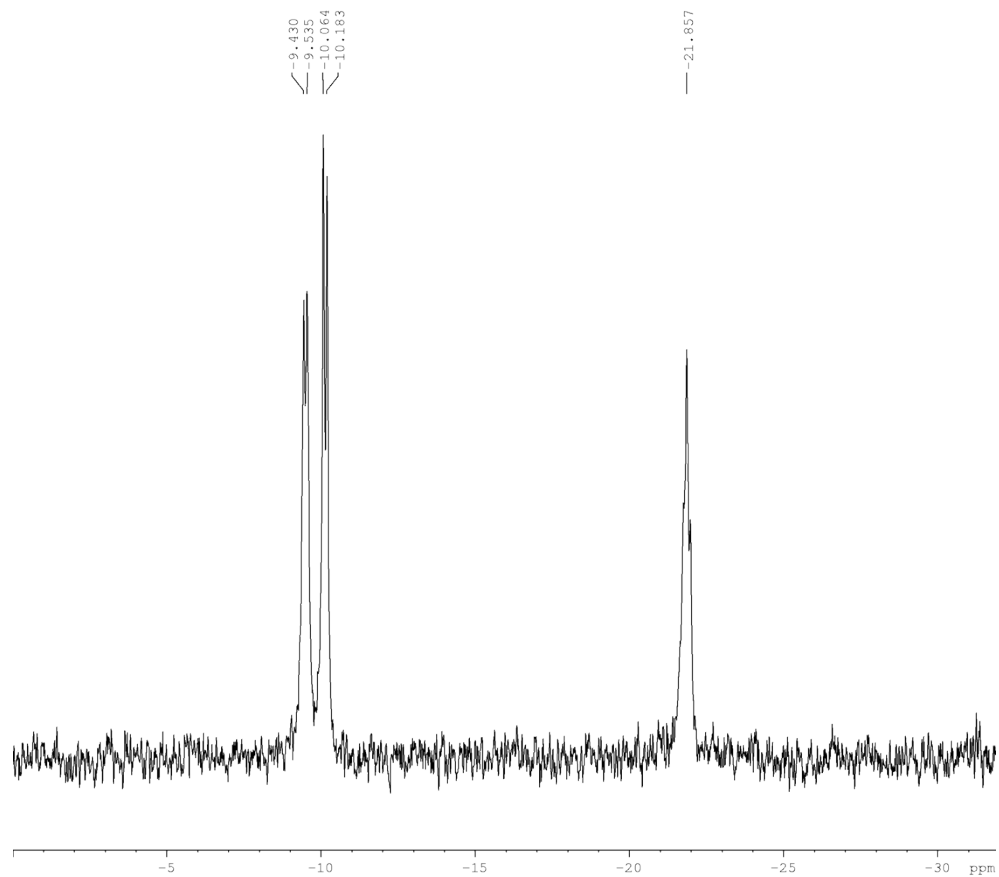
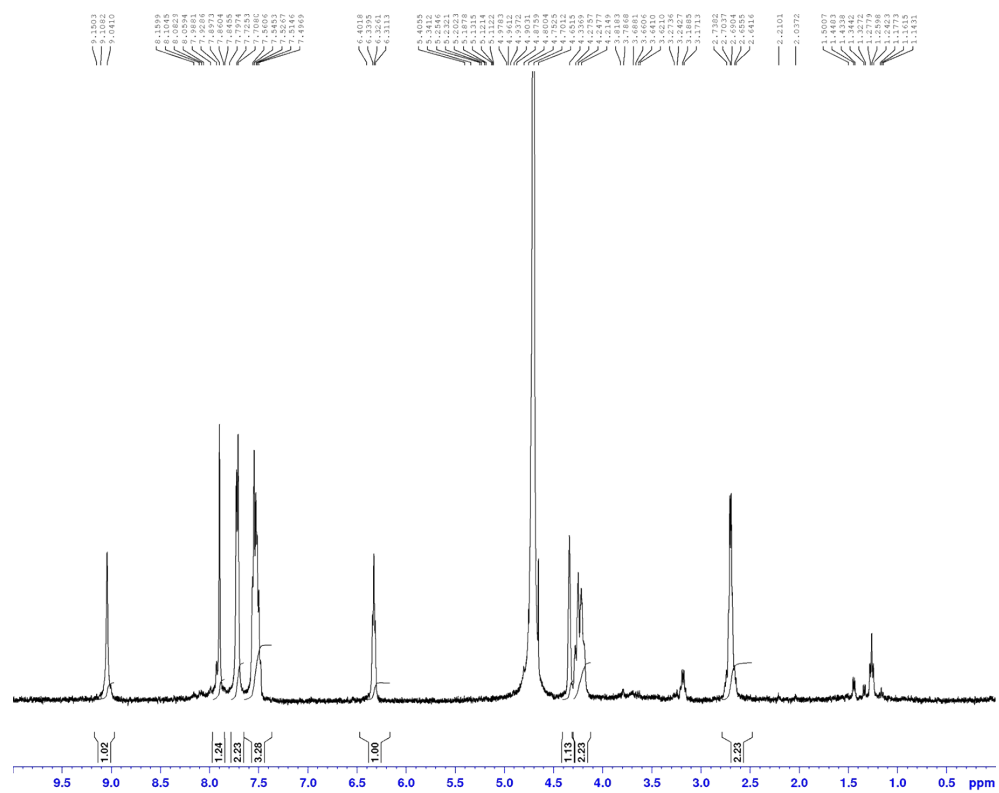


Compound 1 (I)

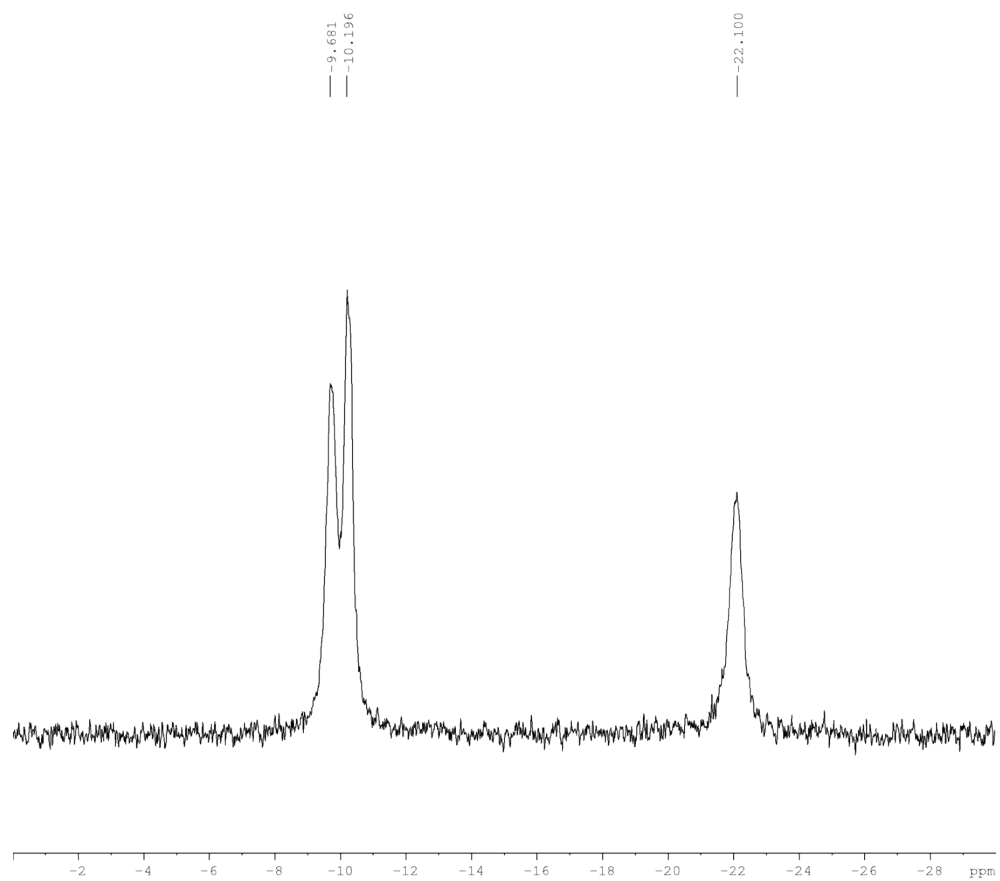
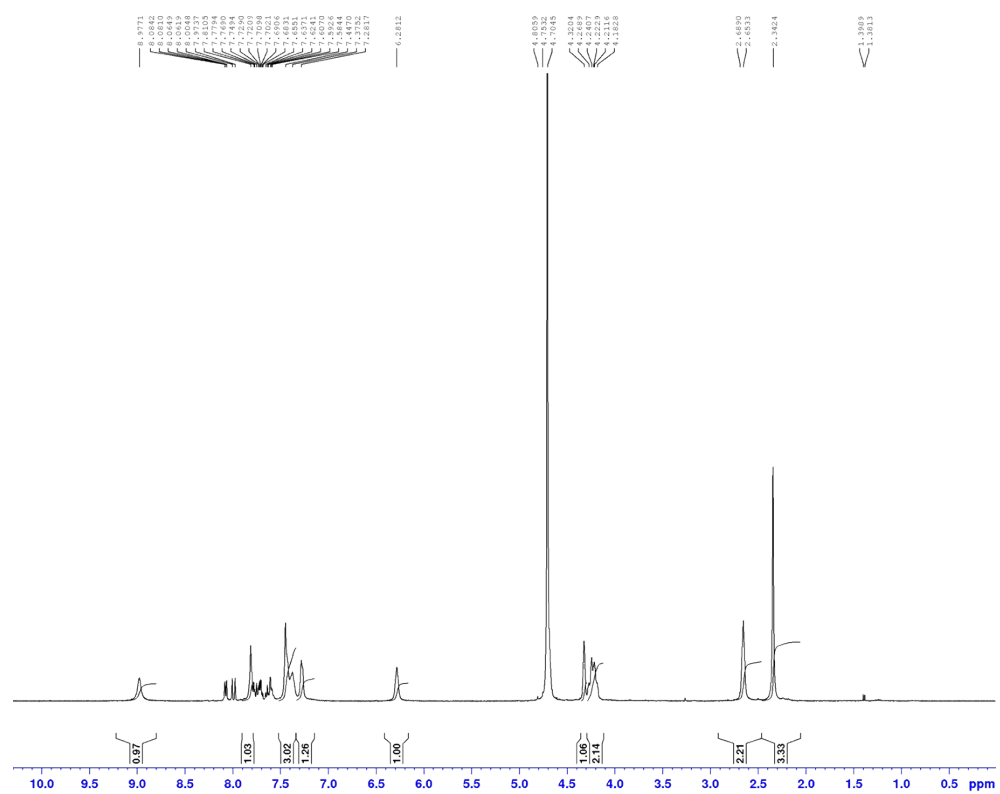




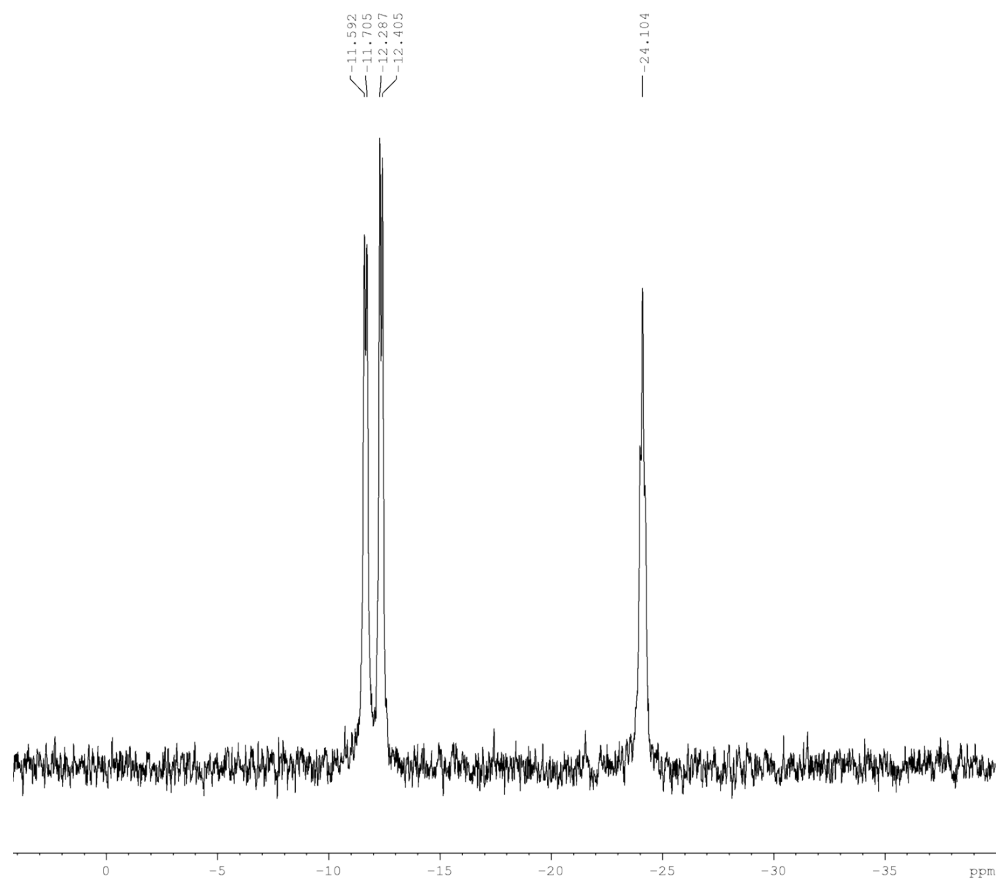
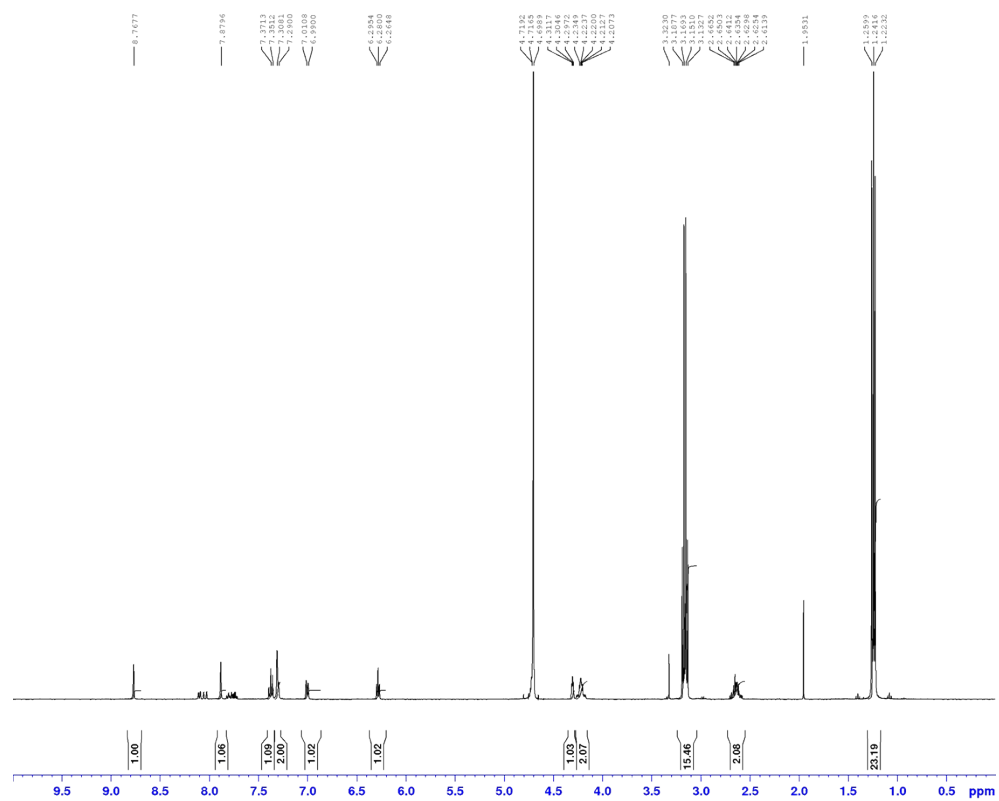
Compound 2 (Ph)



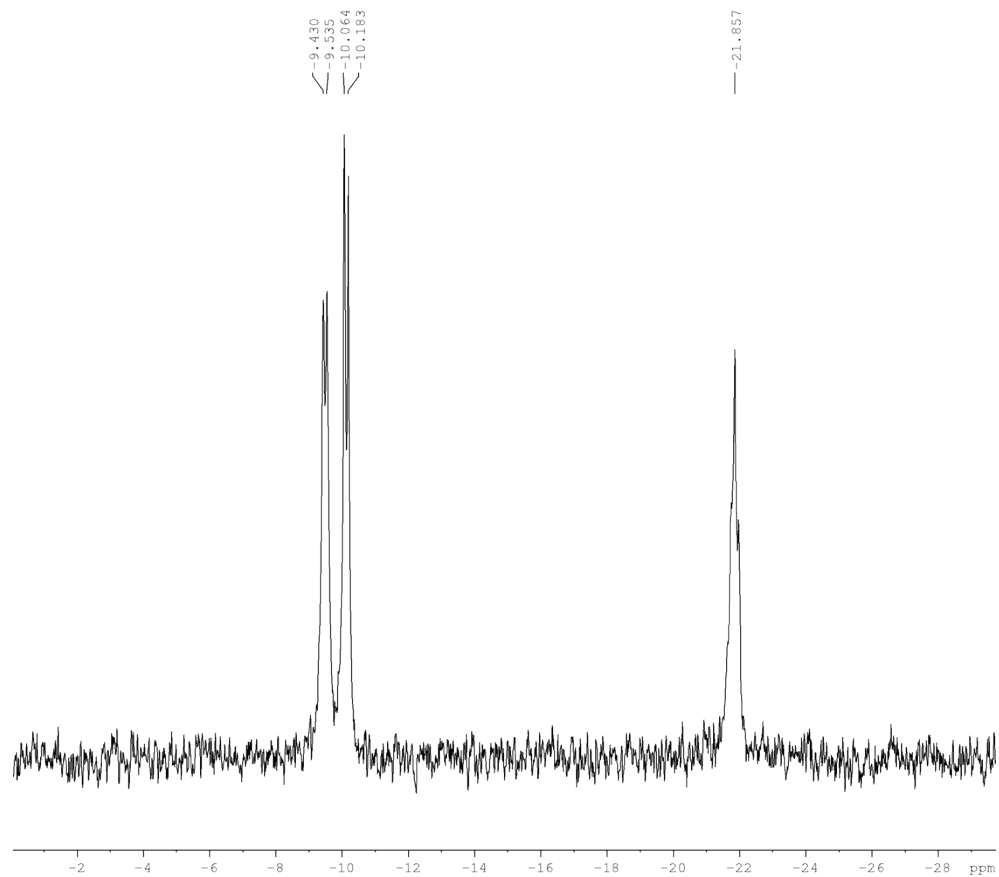
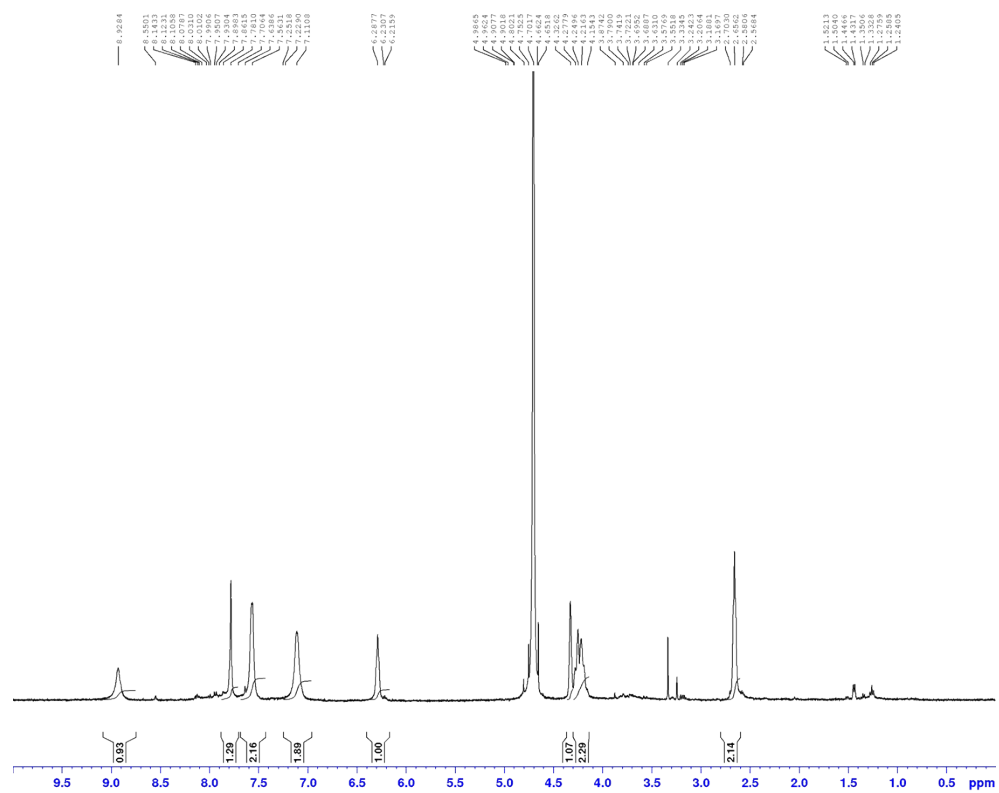
Compound 3 (3MPH)



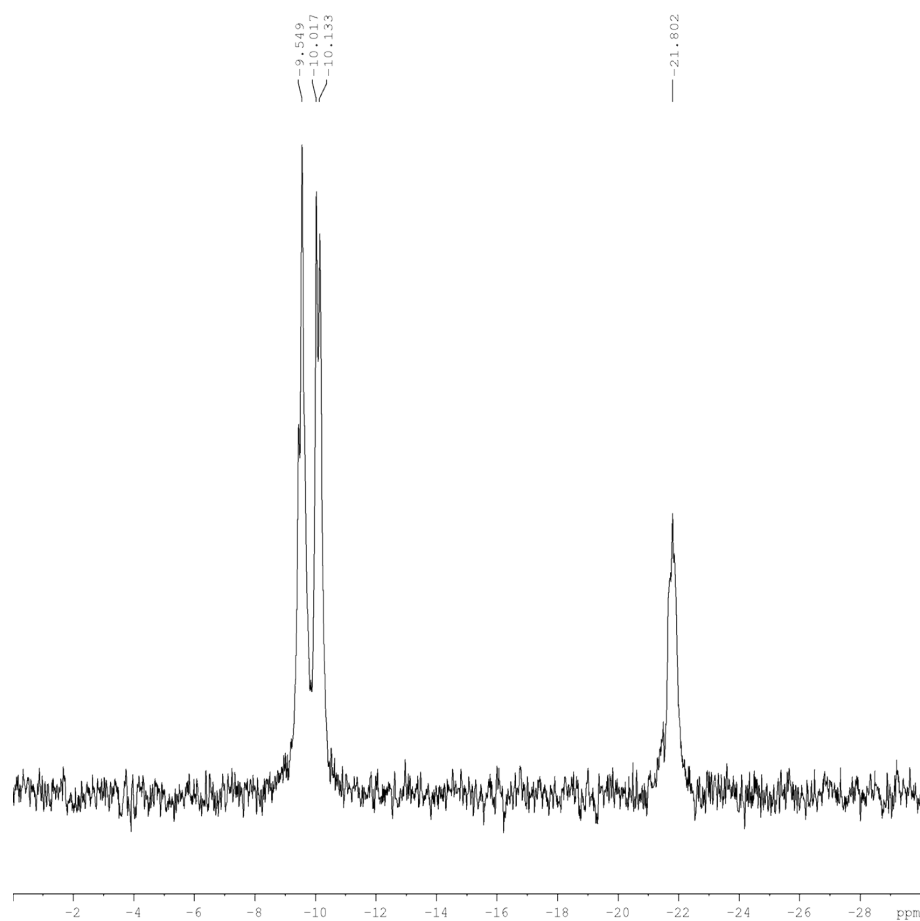
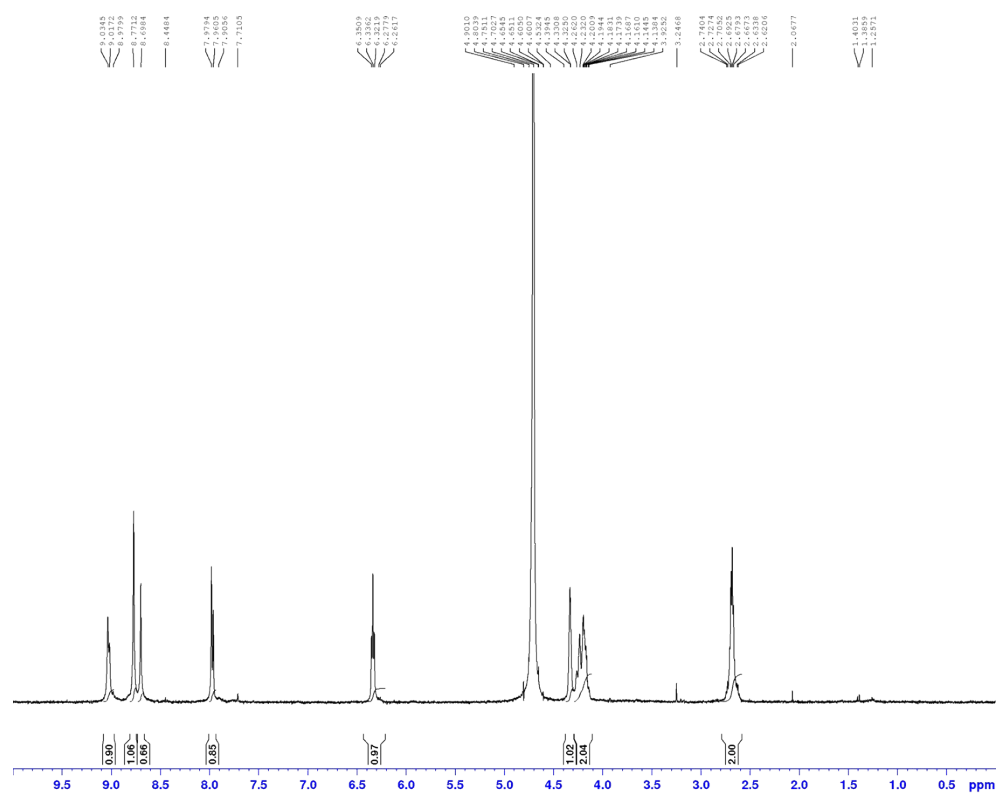
Compound 4 (3APh)



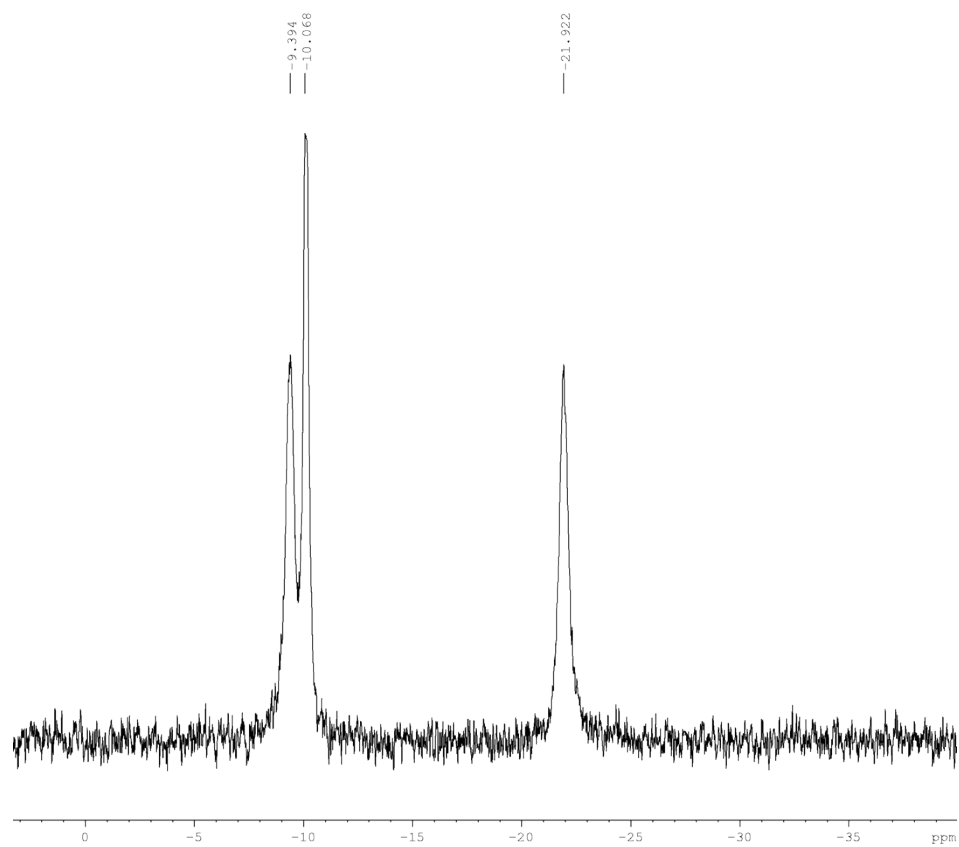
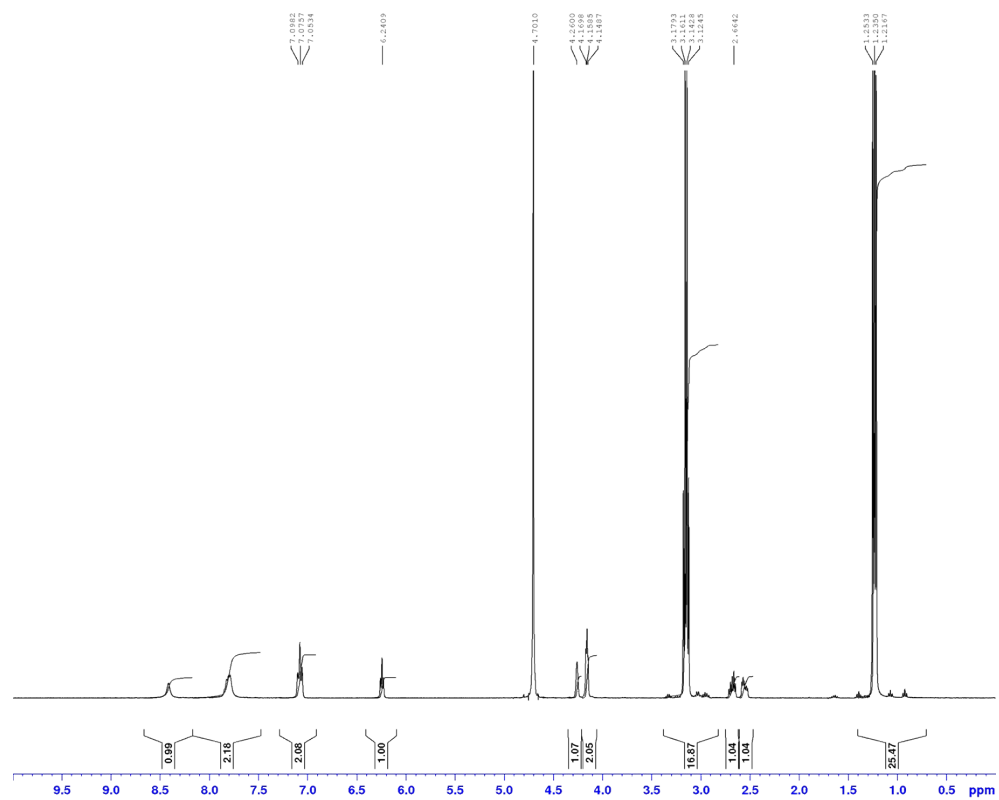
Compound 5 (4APh)



Compound 6 (2APyr)



Compound 7 (2,4FPh)



Compound 8 (2,4OPyr)

