# Electronic Supplementary Information

# Novel Nucleobase-Simplified Cyclic ADP-Ribose Analogue: A Concise Synthesis and $Ca^{2+}$-Mobilizing Activity in T-Lymphocytes

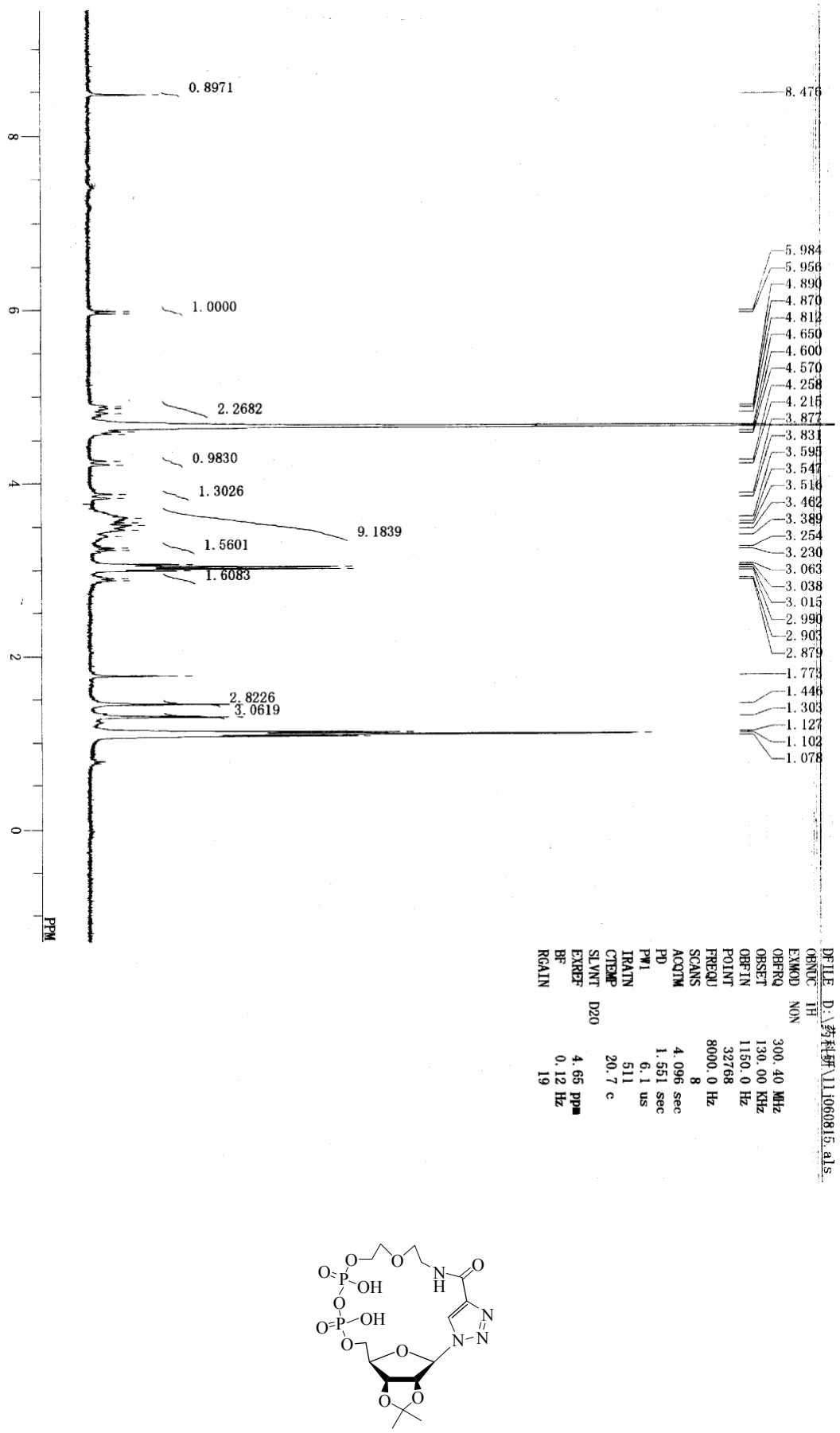
Lingjun Li, [1, 2] † Cornelia C. Siebrands[3] †, Zhenjun Yang,[1] Liangren, Zhang,[1] Andreas H. Guse[3] and Lihe Zhang[1]*

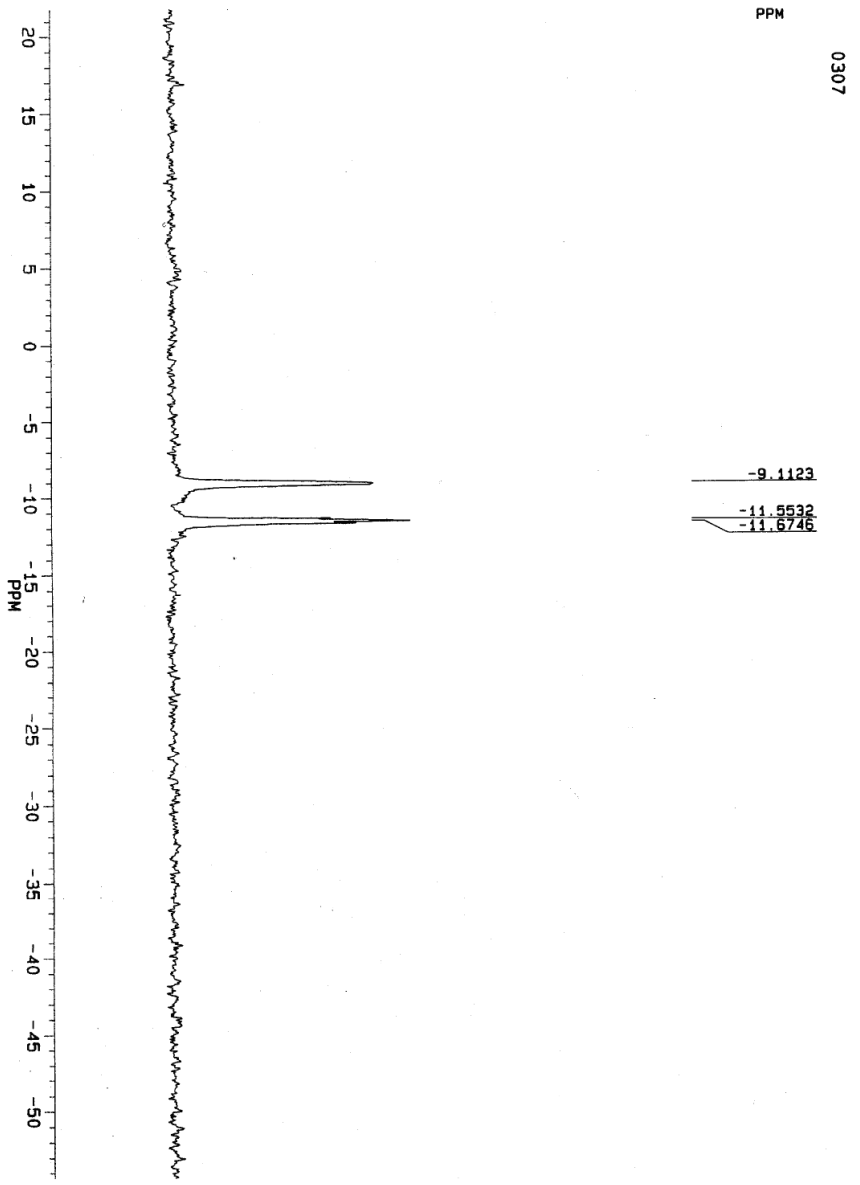
[1] *National Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Sciences, Peking University, Beijing 100083, P.R. China*

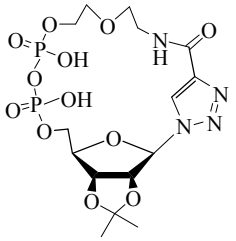
[2] *College of Chemistry and Environmental Science, Henan Normal University, Xinxiang 453007, P.R. China*

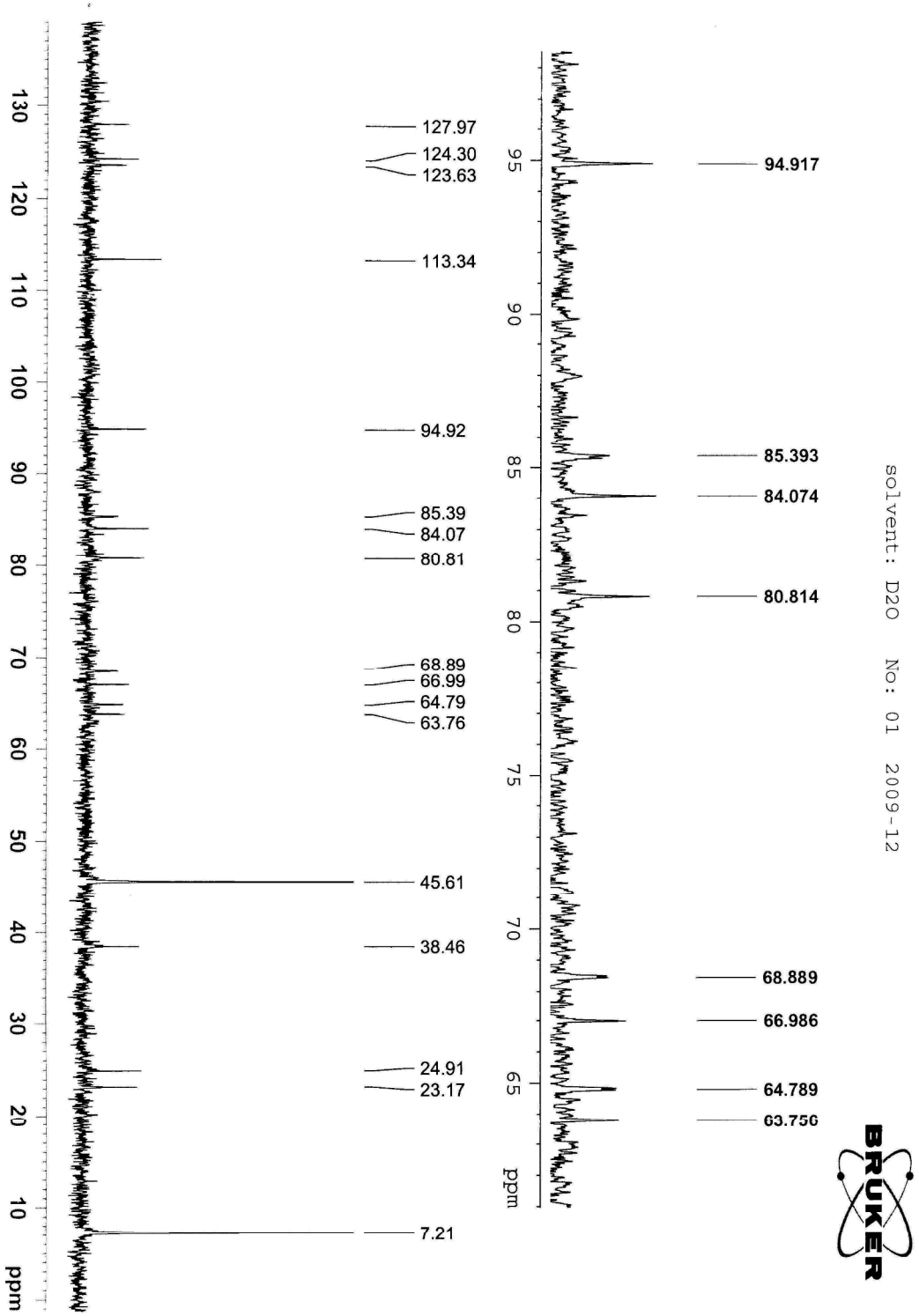
[3]*The Calcium Signaling Group, University Medical Center Hamburg-Eppendorf, Center of Experimental Medicine, Institute of Biochemistry and Molecular Biology I: Cellular Signal Transduction, 20246 Hamburg, Germany*

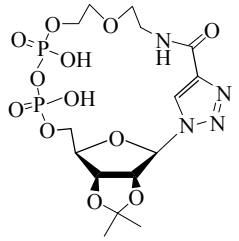
$^1$H NMR and $^{13}$C NMR data were recorded with a JEOL AL300, Avance 400/DPX (Bruker) or a Varian VXR-500 spectrometer using DMSO-*d*6, $CD_3OD$, $CDCl_3$ or $D_2O$ as solvent. Chemical shifts are reported in parts per million downfield from TMS ($^1$H and $^{13}$C). $^{31}$P NMR spectra were recorded at room temperature by use of Bruker Avance 200 spectrometer (81 MHz) and Bruker Avance 300 spectrometer (121.5 MHz); orthophosphoric acid (85%) was used as an external standard. The purity of ompound **6b** was determined by HPLC using the known compound 1H-1,2,3-triazole as a control and compound **6b** prepared by new method ( lot 5) is consistent with the compound reported by us previously (lot 6).

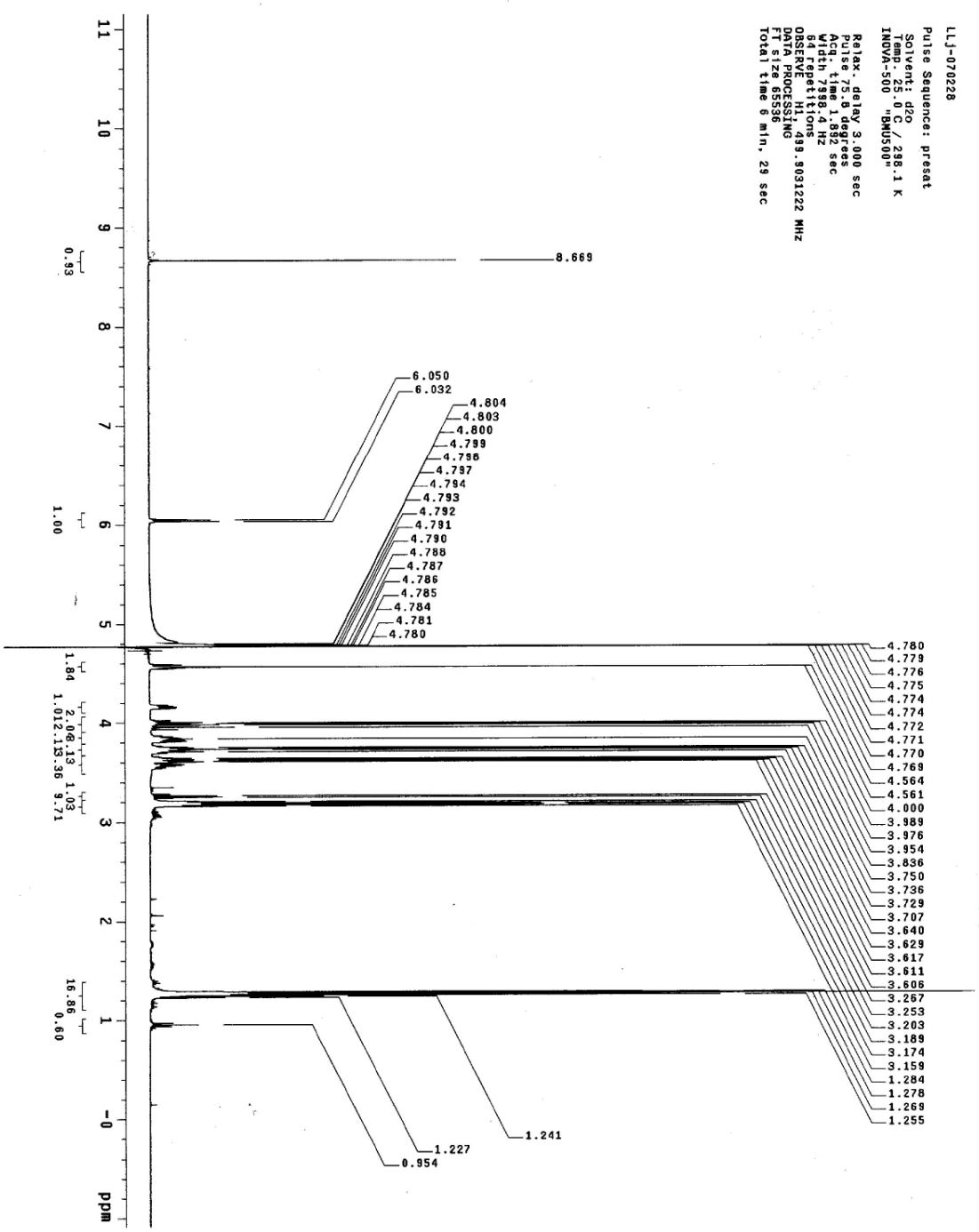


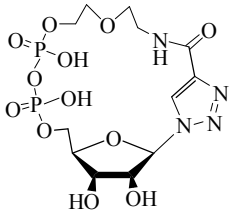


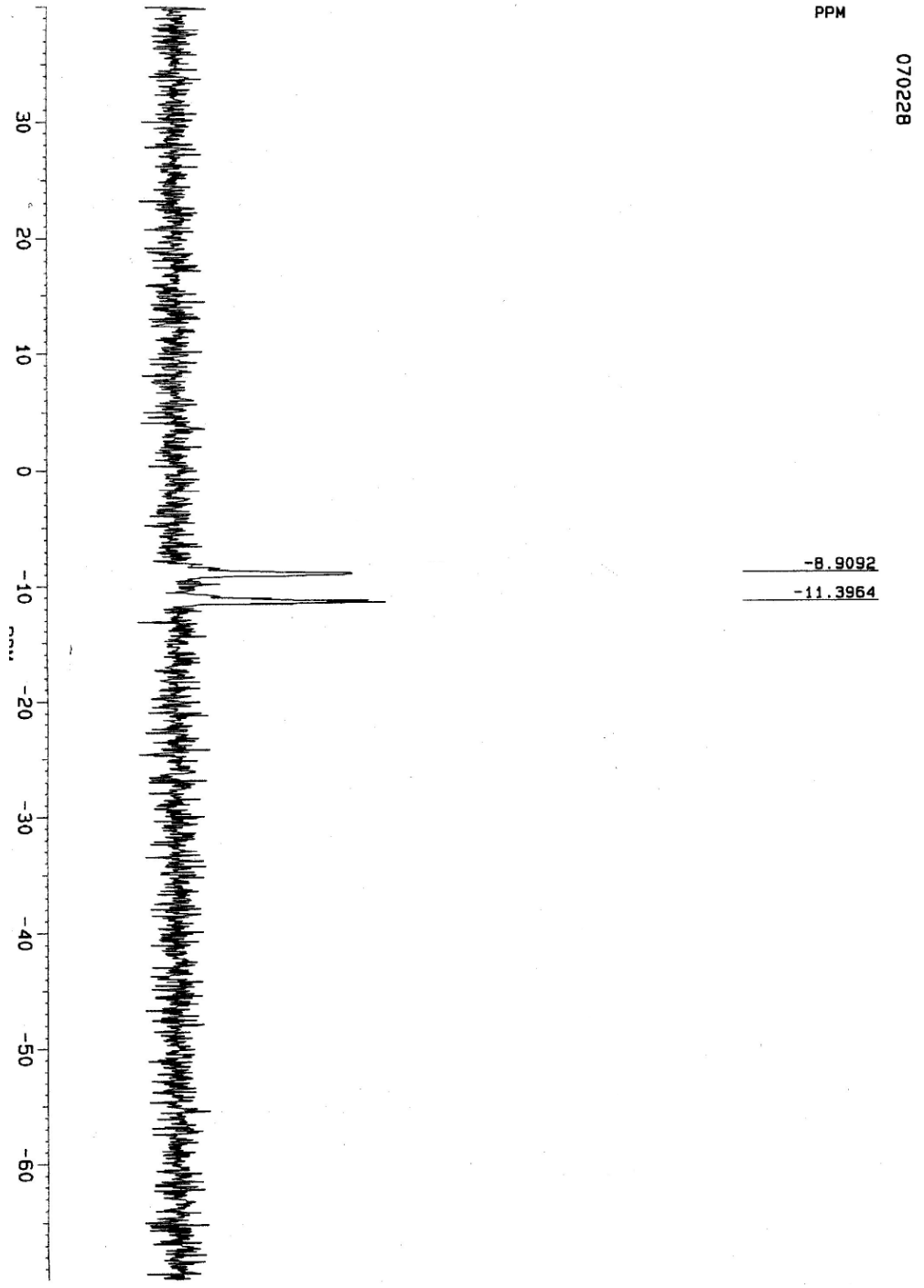



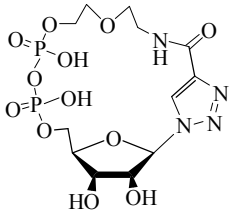


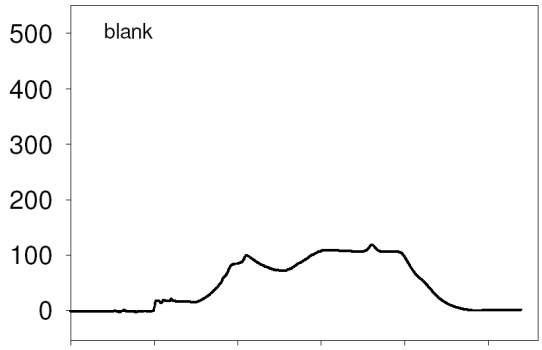


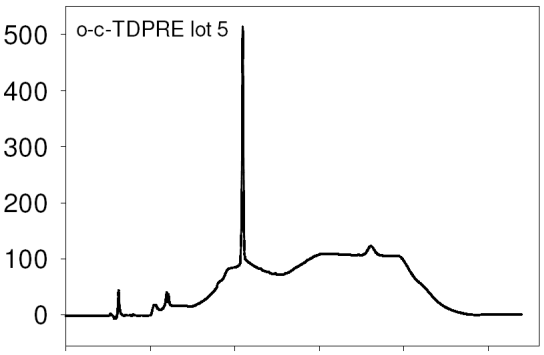





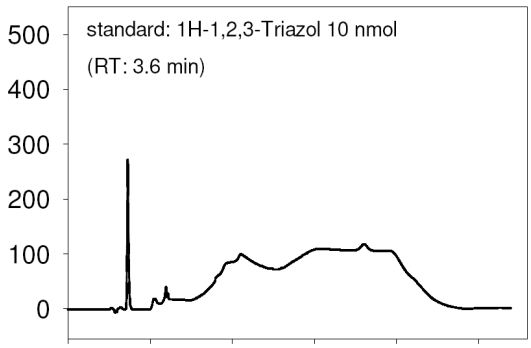



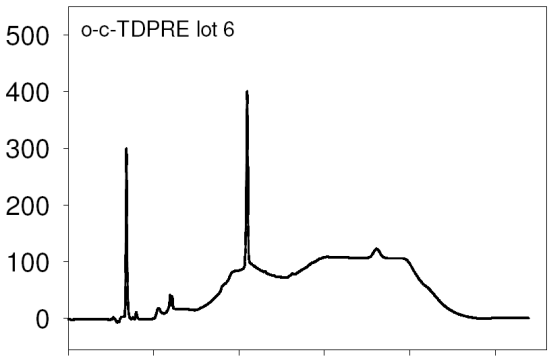
Column: 250 x 4.6 mm Multohyp BDS C 18 - 5 µ
flow: 1 ml/min; detection: DAD detector (205 nm)
buffer A: 20 mM $KH_2PO_4$/ 5 mM TBAHP/ pH 6; buffer B: buffer A with 50 % methanol;
gradient (% buffer B): 0 min (30), 3.5 min (30), 5.5 min (65), 6.5 min (65), 9 min (80), 11 min (100),
16 min (100), 18 min (30), 27 min (30);




o-c-TDPRE lot5
RT: 10.5 min
calculated with reference
to Triazol: 77 mM
expected: 50mM




o-c-TDPRE lot6
RT: 10.5 min
calculated with reference
to Triazol: 56 mM
expected: 50mM;
additional peak: 3.4 min