

Supporting Information
for
Two strategies for the synthesis of the biologically important ATP
analogue ApppI, at a multi-milligram scale

Janne Weisell, Jouko Vepsäläinen and Petri A. Turhanen*

Address: University of Eastern Finland, School of Pharmacy, Biocenter Kuopio, P.O.
Box 1627, FIN-70211, Kuopio, Finland

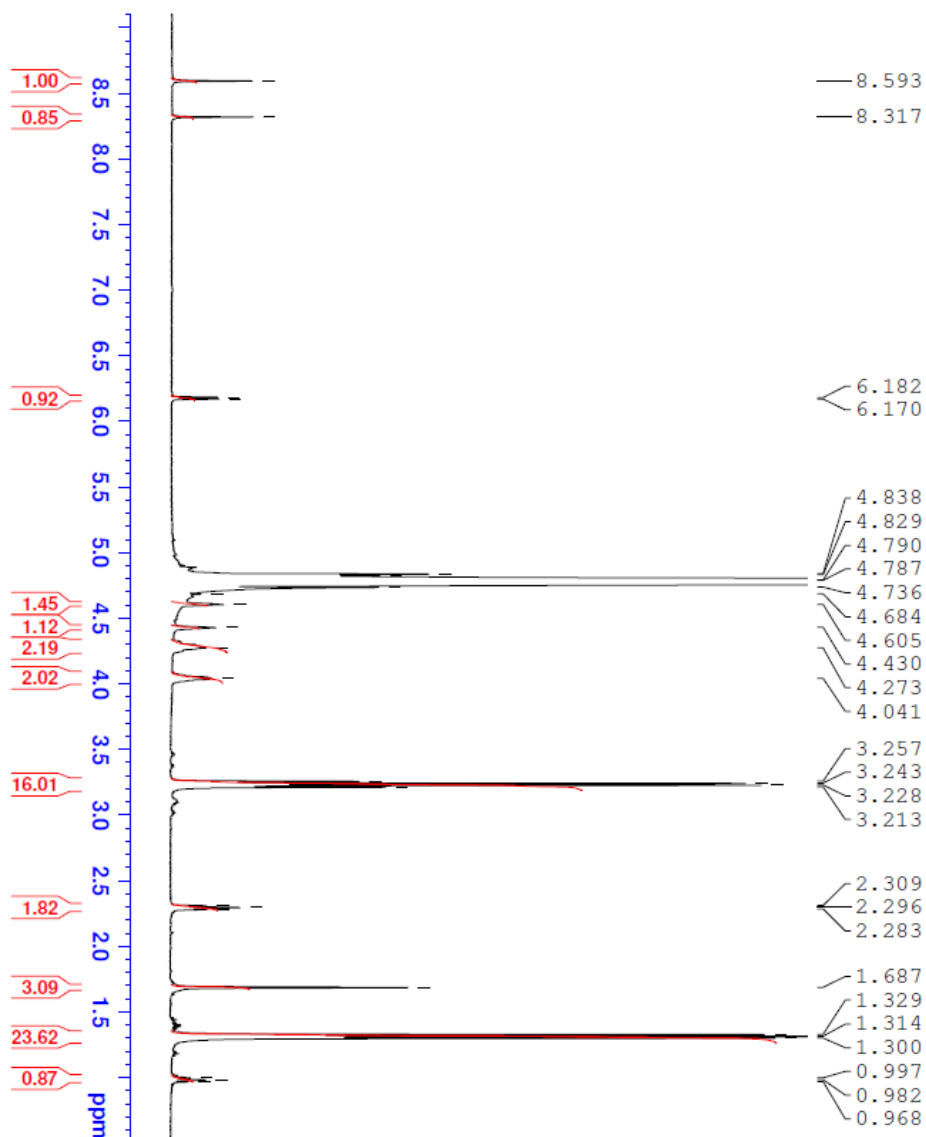
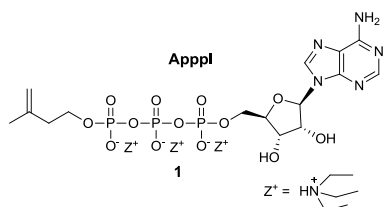
Email: Petri A. Turhanen - petri.turhanen@uef.fi

*Corresponding author

^1H , ^{13}C and ^{31}P NMR spectra for ApppI (1) and typical example of
HPLC chromatogram of ApppI purification

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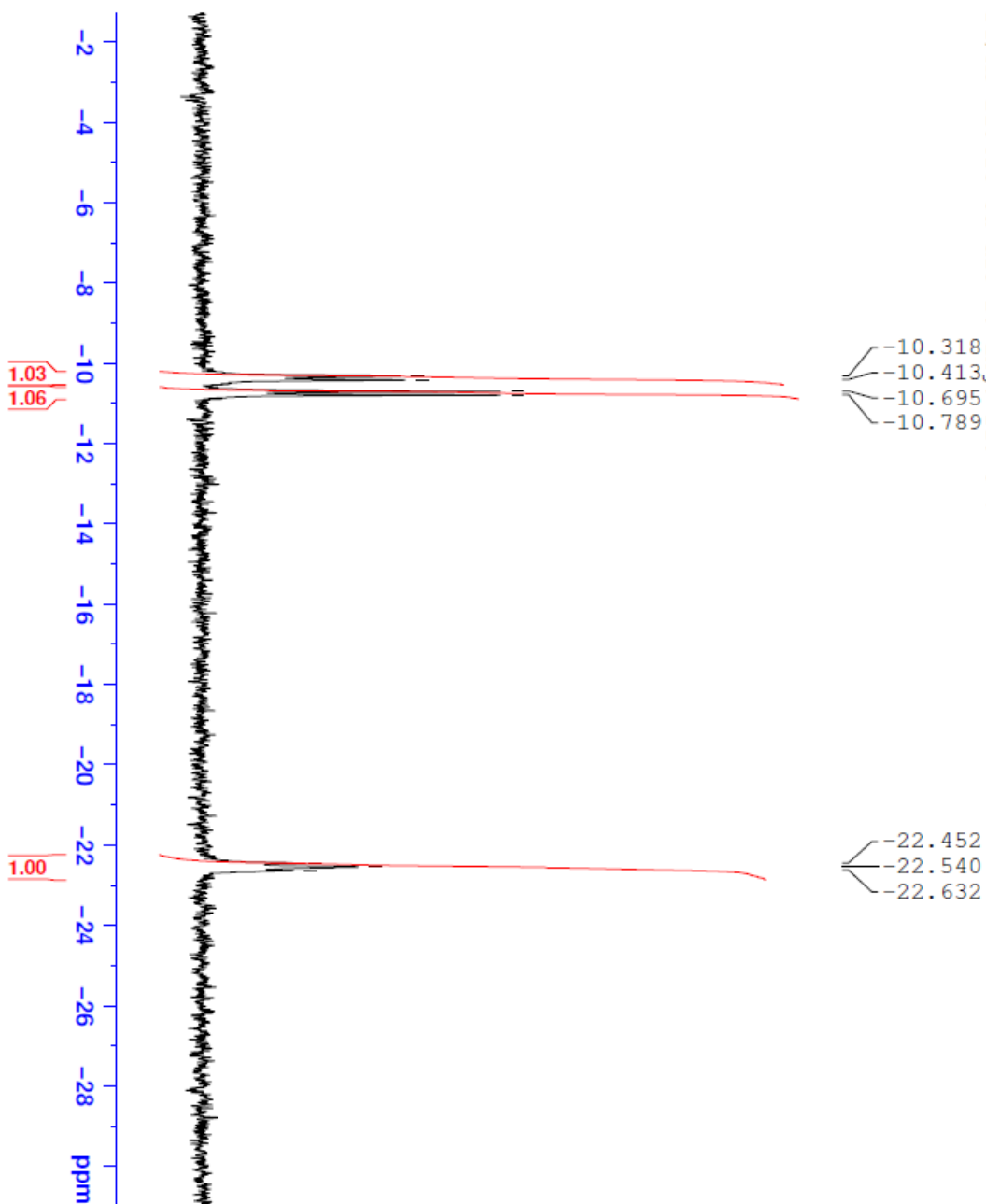
BRUKER

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SOLVENT    D2O
NS         32
DS         0
SWH        10000.000 H
FIDRES     0.152588 H
AQ         3.2769001 s
RG          64
DE         50.000 u
TE         6.00 u
D1         300.0 K
D10        5.00000000 s
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         10.06 u
PL1        -1.00 d
SFO1       500.1340010 M
SI         262144
SF         500.129575 M
WDW        EM
SSB        0
LB         0.30 H
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PT/MS-220413-3a d2o 1. inj. fr. 6-7



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SOLVENT   D2O
NS         80
DS         0
SWH        40650.406 H
FIDRES     0.620276 H
AQ         0.8061551 s
RG         2048
DW         12.300 u
DE         6.00 u
TE         300.0 K
D1         2.00000000 s
d11        0.03000000 s
TD0        1

===== CHANNEL f1 =====
NUC1       31P
P1         8.50 u
PL1        10.00 d
SFO1       202.4586930 M

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 u
PL2        -1.00 d
PL12       18.00 d
SFO2       500.1325007 M
SI         262144
SF         202.4561723 M
WDW        EM
SSB        0
GB         2.00 H
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PT/MS-220413-3a d2o tsp 1. inj. fr. 6-7

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155.71
152.09
146.25
142.78

121.58
114.18

89.58
86.99
86.91

77.20
73.29
68.09
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67.56

49.56

40.58
40.53

24.51

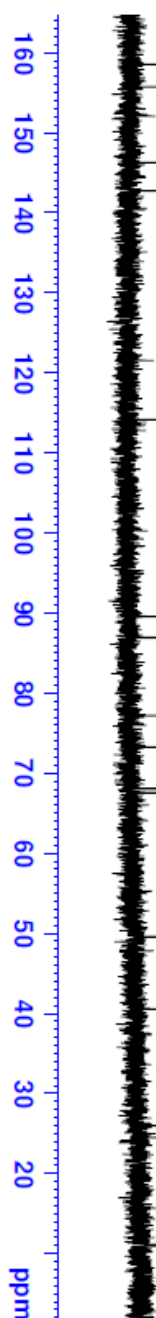
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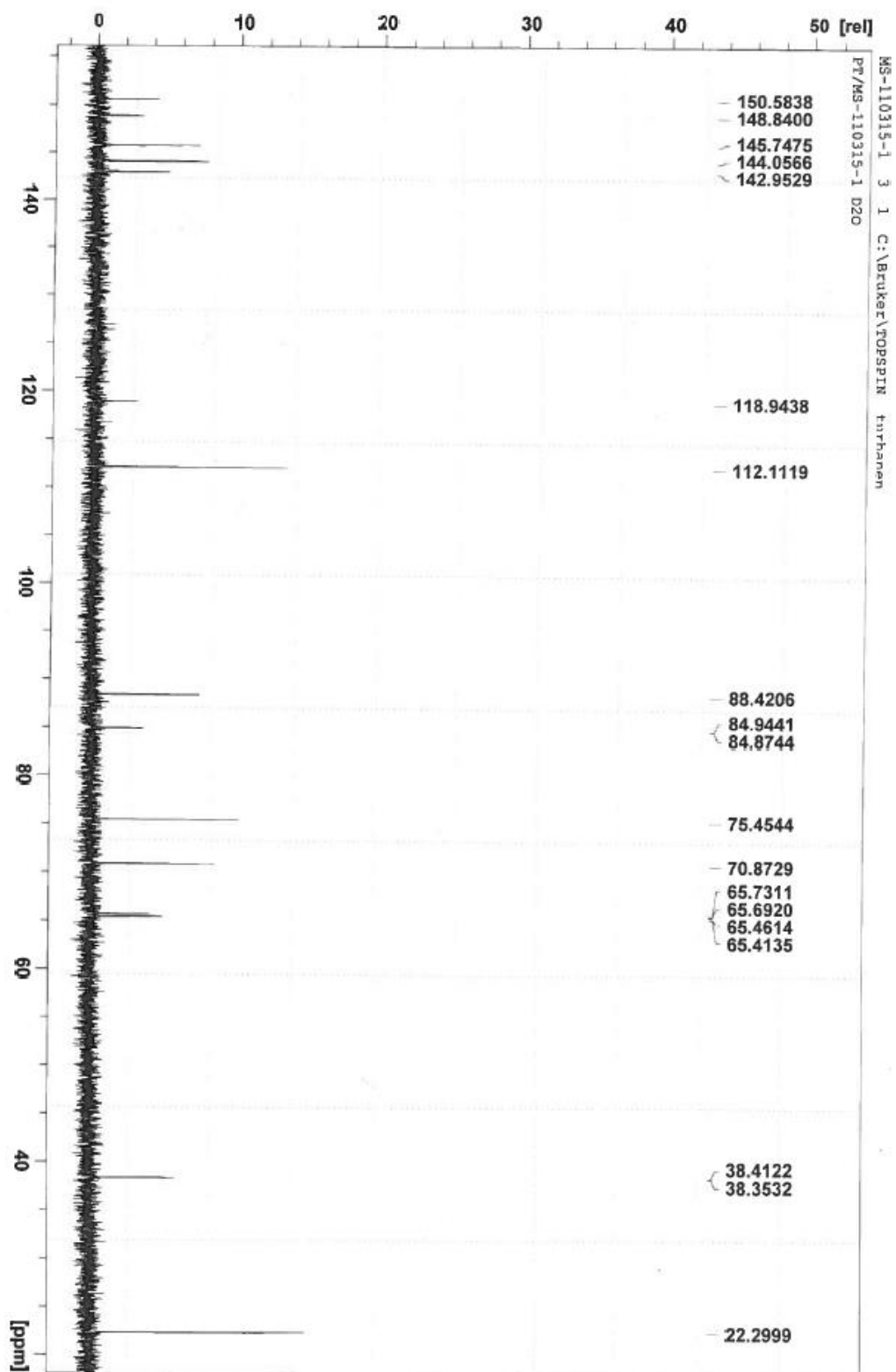


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SOLVENT MeOD
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FIDRES 0.231194 Hz
AQ 2.1627545 sec
RG 8192
DM 16.500 use
DE 6.00 use
TE 300.0 K
D1 20.00000000 sec
d11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
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P1 8.75 use
PL1 6.00 dB
SFO1 125.7715724 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 90.00 use
PL2 -1.00 dB
PL12 18.00 dB
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SI 524288
SF 125.7572328 MHz
WDW EM
SSB 0
LB 1.20 Hz
GB 0
PC 0.90



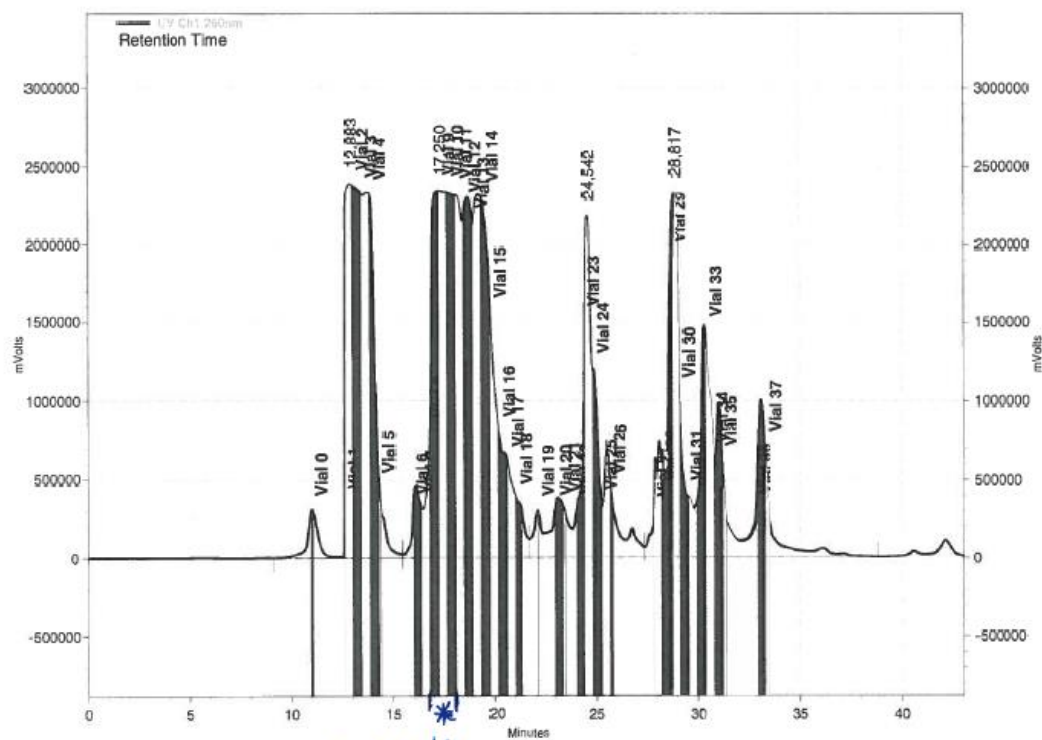


BMG

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46min.met
User: Ale Närvänen
Analysed: 3.12.2013 9:42:26



1-4 + 41-44 2.8059
8-10 5.1519 → AappI
11-16 5.2023