



## Supporting Information

for

### Synthesis of the biologically important dideuterium-labelled adenosine triphosphate analogue Apppl( $d_2$ )

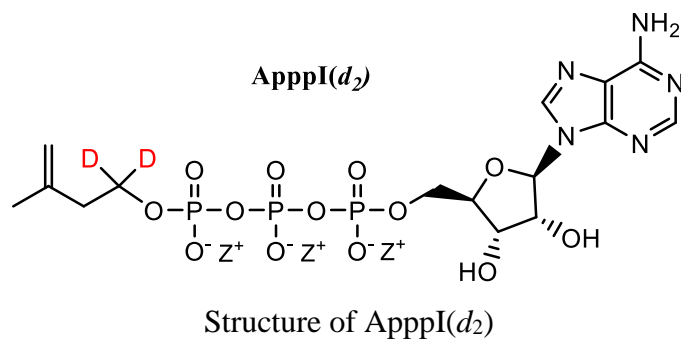
Petri A. Turhanen

*Beilstein J. Org. Chem.* **2022**, *18*, 1466–1470. [doi:10.3762/bjoc.18.153](https://doi.org/10.3762/bjoc.18.153)

### $^1\text{H}$ , $^{13}\text{C}$ , and $^{31}\text{P}$ NMR spectra as well as HPLC chromatogram of Apppl( $d_2$ ) purification

## Table of contents

Structure of ApppI( <i>d</i> <sub>2</sub> ) .....	S1
<sup>1</sup> H, <sup>31</sup> P, and <sup>13</sup> C NMR spectra of ApppI( <i>d</i> <sub>2</sub> )-3.25 TBA salt .....	S2
Typical HPLC chromatogram for the purification of ApppI( <i>d</i> <sub>2</sub> ) .....	S4



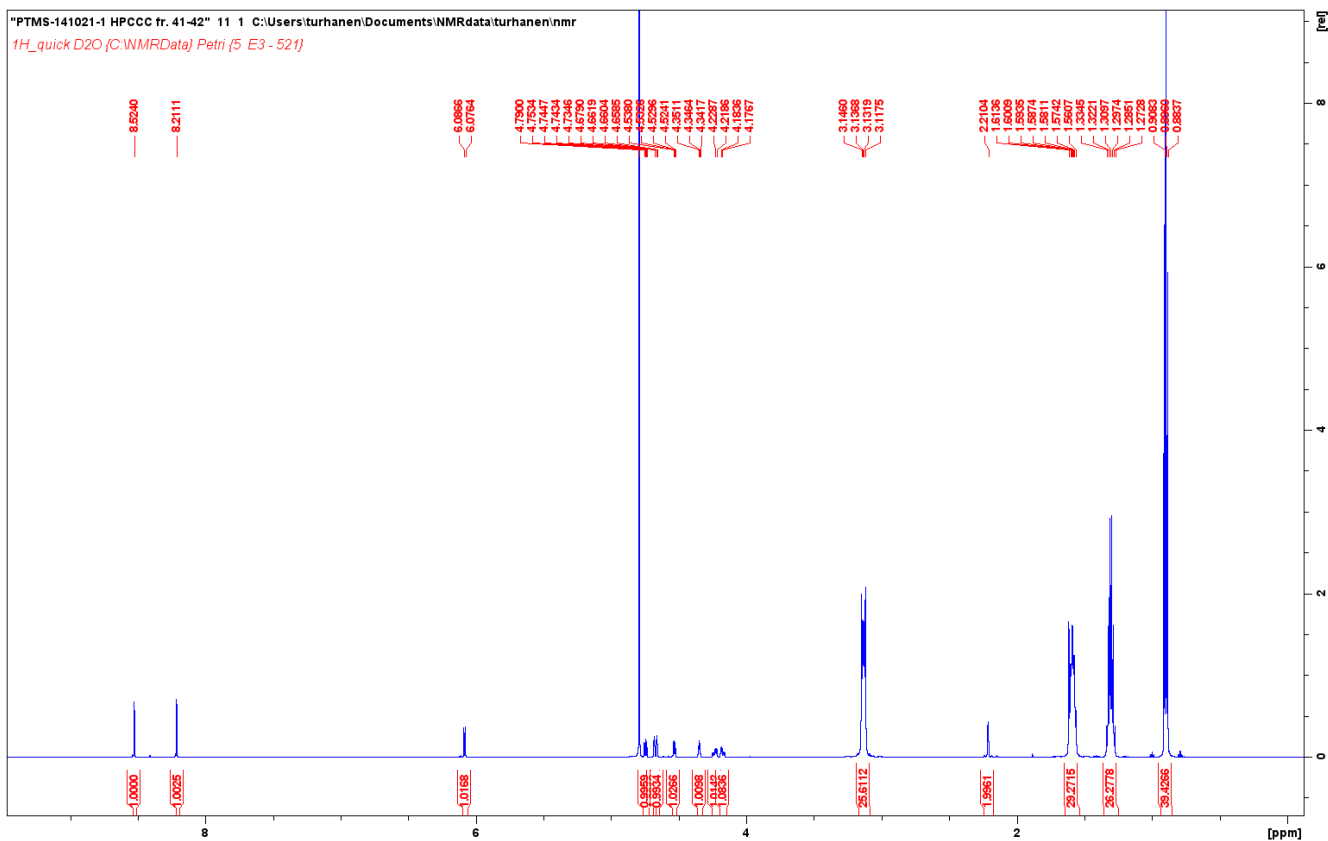


Figure S1:  $^1\text{H}$  NMR spectrum of AppI( $d_2$ )·3.25 TBA salt.

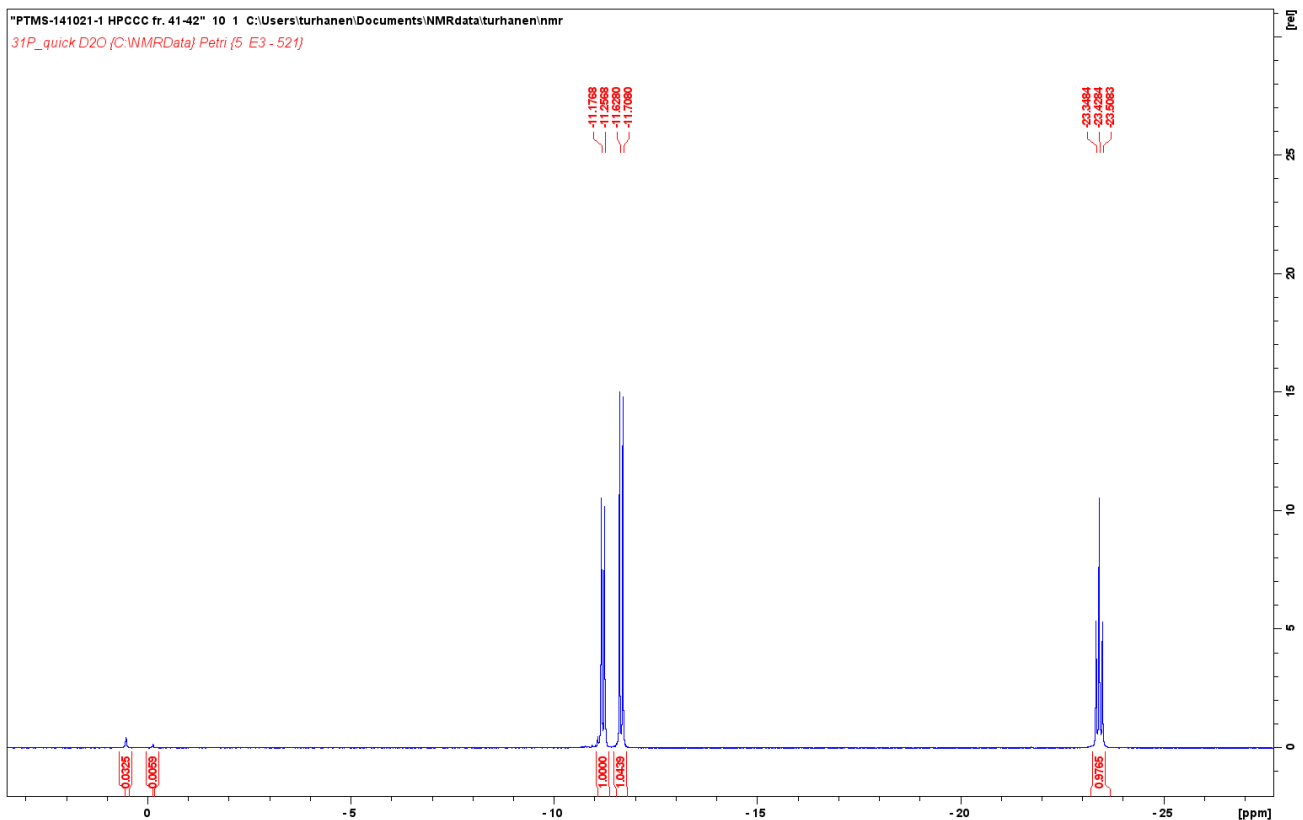
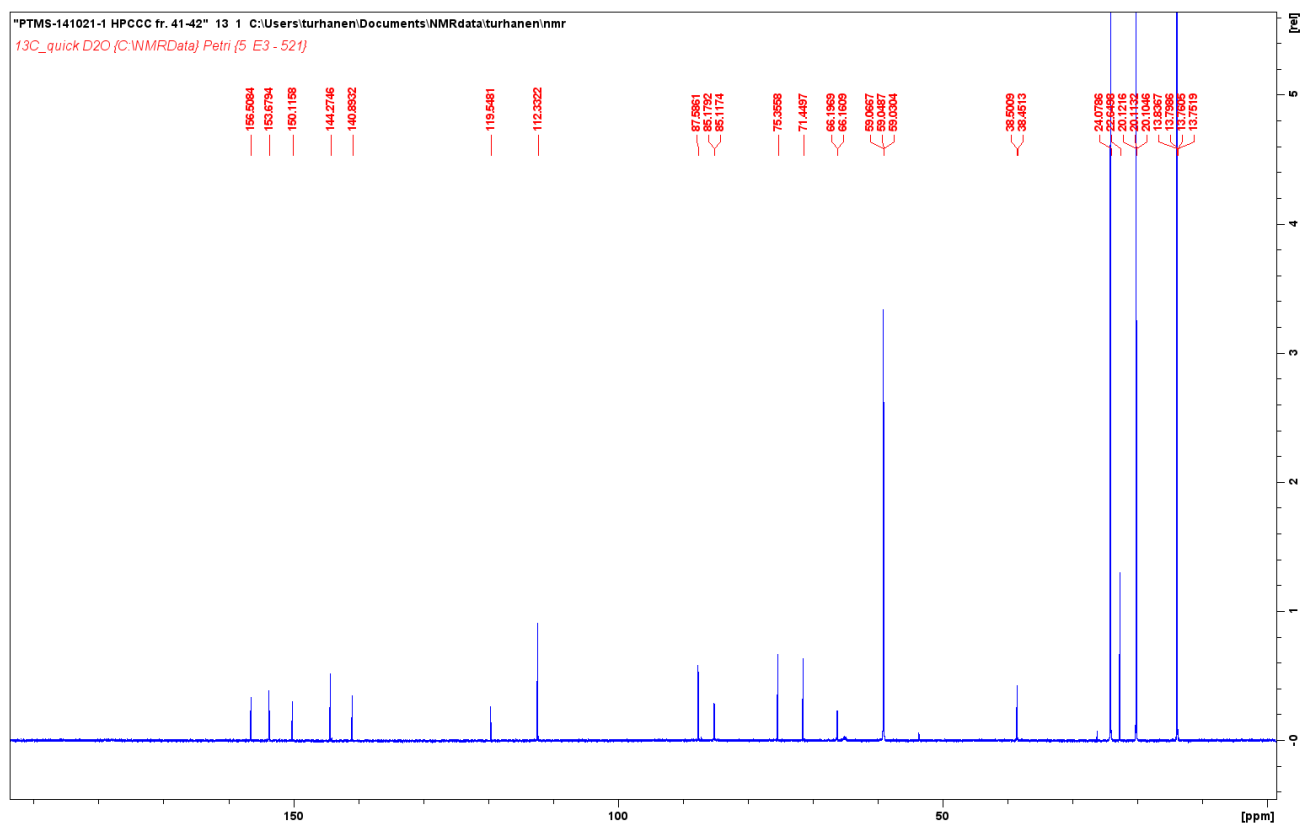
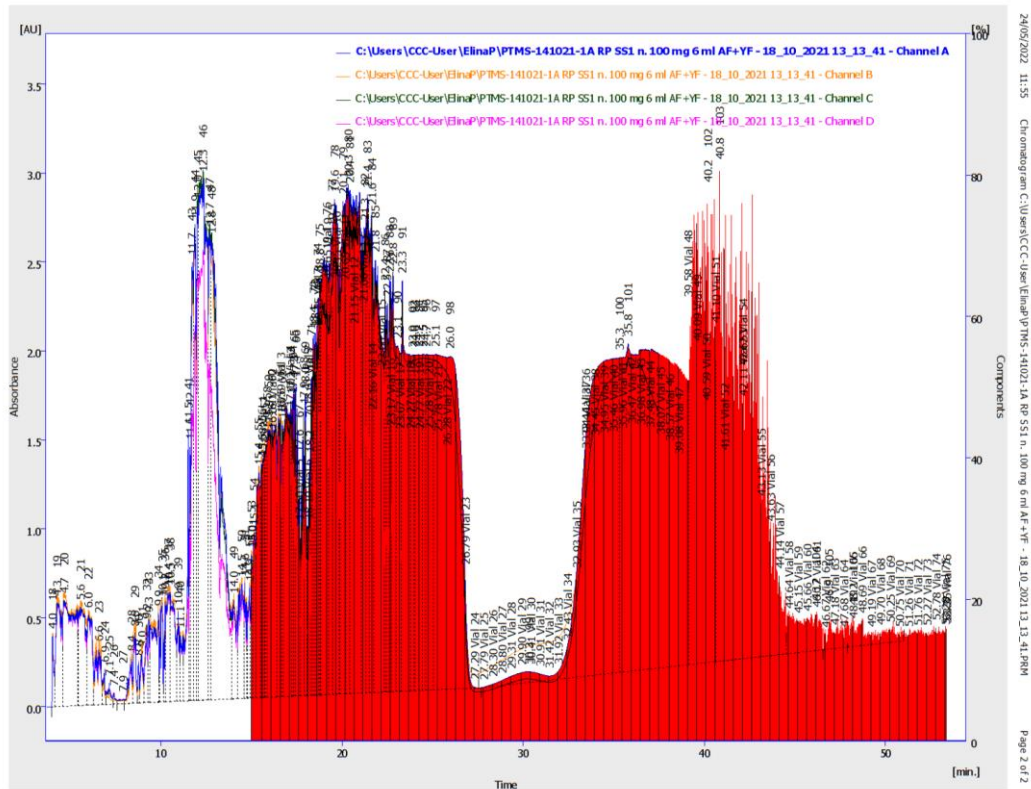


Figure S2:  $^{31}\text{P}$  NMR spectrum of AppI( $d_2$ )·3.25 TBA salt.



**Figure S3:**  $^{13}\text{C}$  NMR spectrum of ApppI( $d_2$ )·3.25 TBA salt.



**Figure S4:** HPLC chromatogram for the purification of AppI( $d_2$ ). Vials 34–40 contained AppI( $d_2$ )·5.25 TBA salt and vials 41–42 AppI( $d_2$ )·3.25 TBA salt.