

Supplementary Materials

# New Chemical Probe Targeting Bacterial NAD Kinase

David A. Clément <sup>1,2,†</sup>, Clarisse Leseigneur <sup>2,3,†</sup>, Muriel Gelin <sup>4,†</sup>, Dylan Coelho <sup>1</sup>, Valérie Huteau <sup>1</sup>, Corinne Lionne <sup>4</sup>, Gilles Labesse <sup>4,\*</sup>, Olivier Dussurget <sup>2,3,\*</sup> and Sylvie Pochet <sup>1,\*</sup>

<sup>1</sup> Institut Pasteur, Unité de Chimie et Biocatalyse, UMR3523 CNRS, Paris 75015, France; david.clement@pasteur.fr (D.A.C.); dylan.coelho@etu.parisdescartes.fr (D.C.); valerie.huteau@pasteur.fr (V.H.)

<sup>2</sup> Faculté des Sciences, Université de Paris, Sorbonne Paris Cité, Paris 75013, France; clarisse.leseigneur@pasteur.fr

<sup>3</sup> Institut Pasteur, Unité de Recherche *Yersinia*, Paris 75015, France; olivier.dussurget@pasteur.fr

<sup>4</sup> Centre de Biochimie Structurale (CBS), CNRS, INSERM, Université de Montpellier, Montpellier 34090, France; gelin@cbs.cnrs.fr (M.G.); lionne@cbs.cnrs.fr (C.L.)

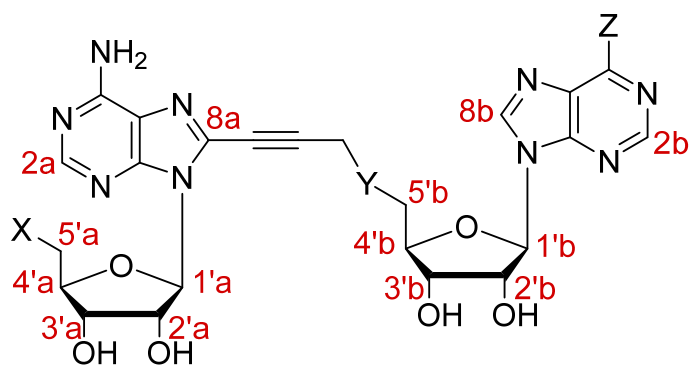
\* Correspondence: labesse@cbs.cnrs.fr (G.L.); olivier.dussurget@pasteur.fr (O.D.); sylvie.pochet@pasteur.fr (S.P.)

† These authors contributed equally to this work.

**Table of contents**

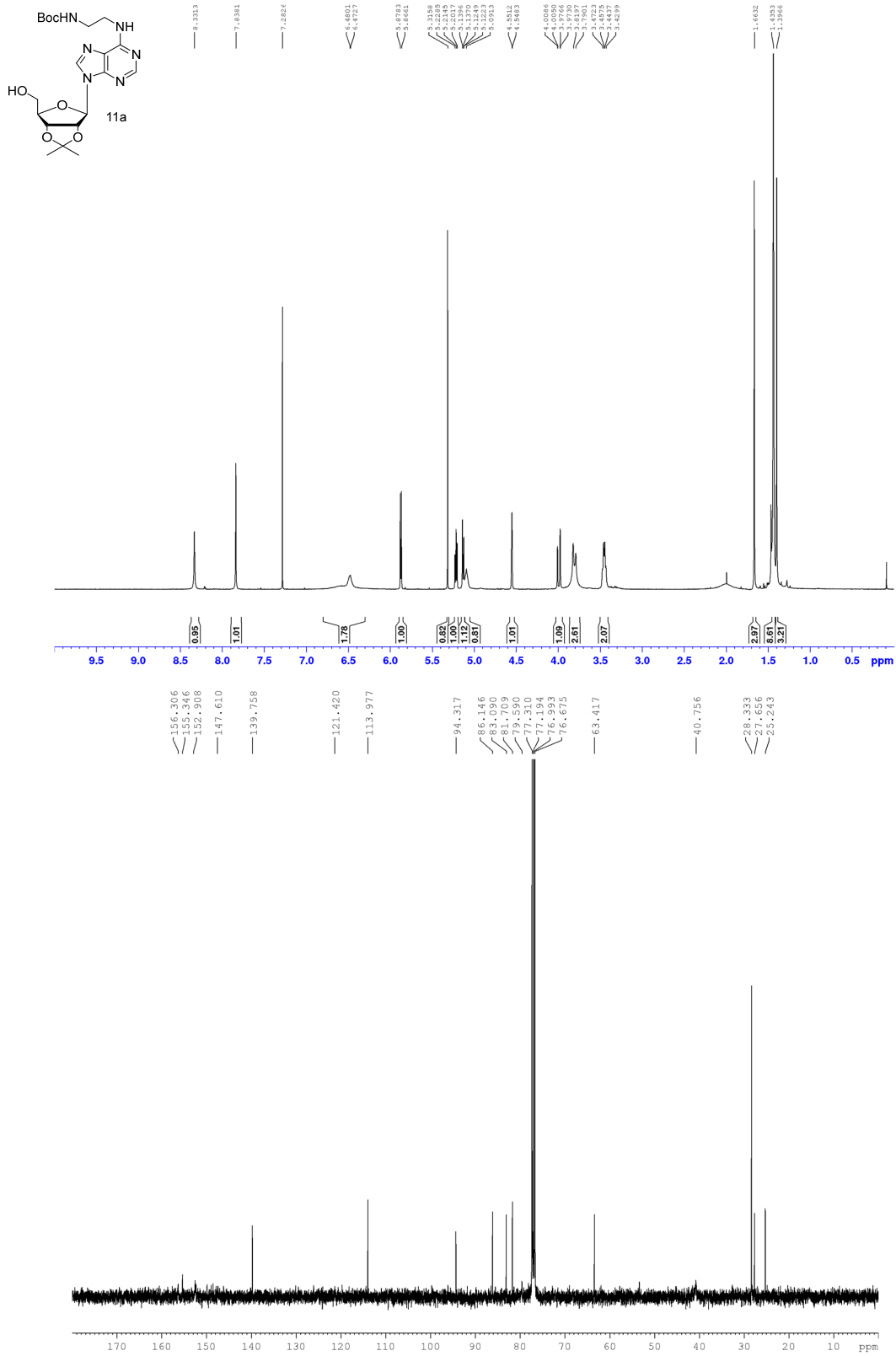
<b>1. Numbering of synthesized molecules .....</b>	<b>3</b>
<b>2. NMR spectra of final compounds.....</b>	<b>4</b>
Compound <b>11a</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	4
Compound <b>11a</b> : HSQC (red) and HMBC (blue) spectra .....	5
Compound <b>11b</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra.....	6
Compound <b>11b</b> : HSQC (red) and HMBC (blue) spectra .....	7
Compound <b>8a</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	8
Compound <b>8a</b> : HSQC (red) and HMBC (blue) spectra .....	9
Compound <b>8b</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra.....	10
Compound <b>8b</b> : HSQC (red) and HMBC (blue) spectra .....	11
Compound <b>12a</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	12
Compound <b>12b</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra.....	13
Compound <b>2</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	14
Compound <b>3</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	15
Compound <b>14</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	16
Compound <b>7</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	17
Compound <b>15</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	18
Compound <b>4</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	19
Compound <b>16</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	20
Compound <b>17</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	21
Compound <b>18</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	22
Compound <b>19</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	23
Compound <b>5</b> : $^1\text{H}$ and $^{13}\text{C}$ spectra .....	24

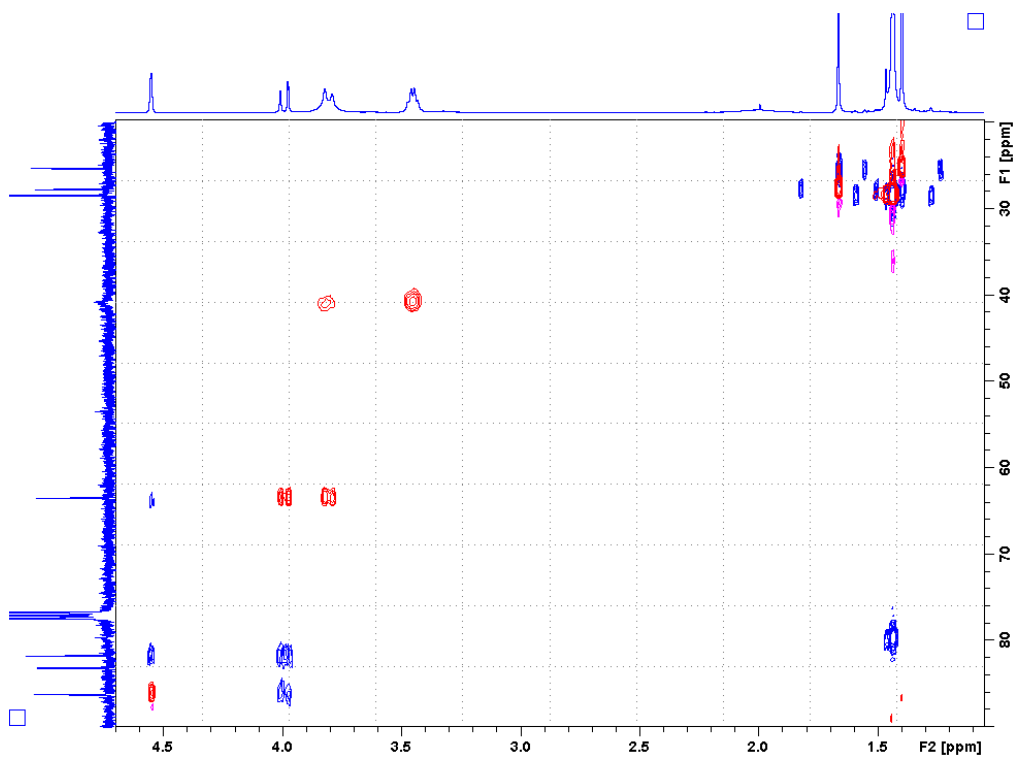
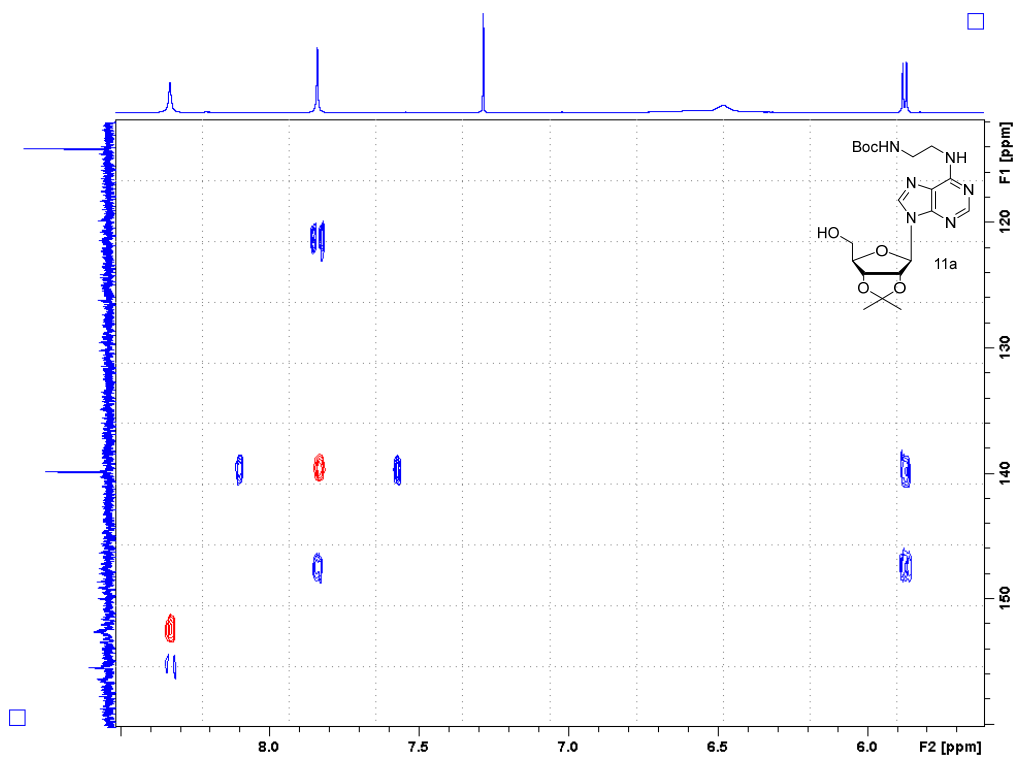
## 1. Numbering of Synthesized Molecules

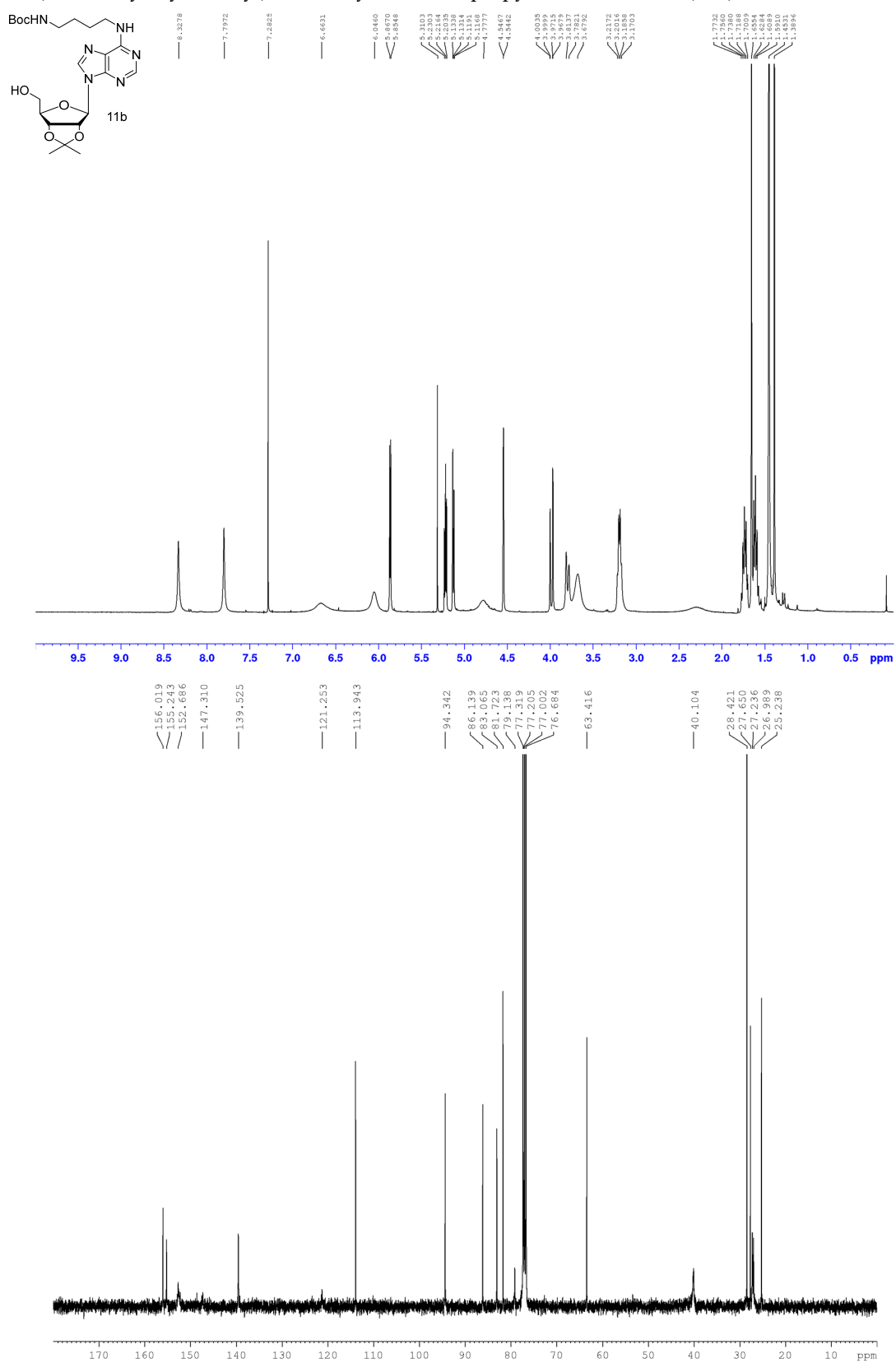


## 2. NMR spectra of Final Compounds

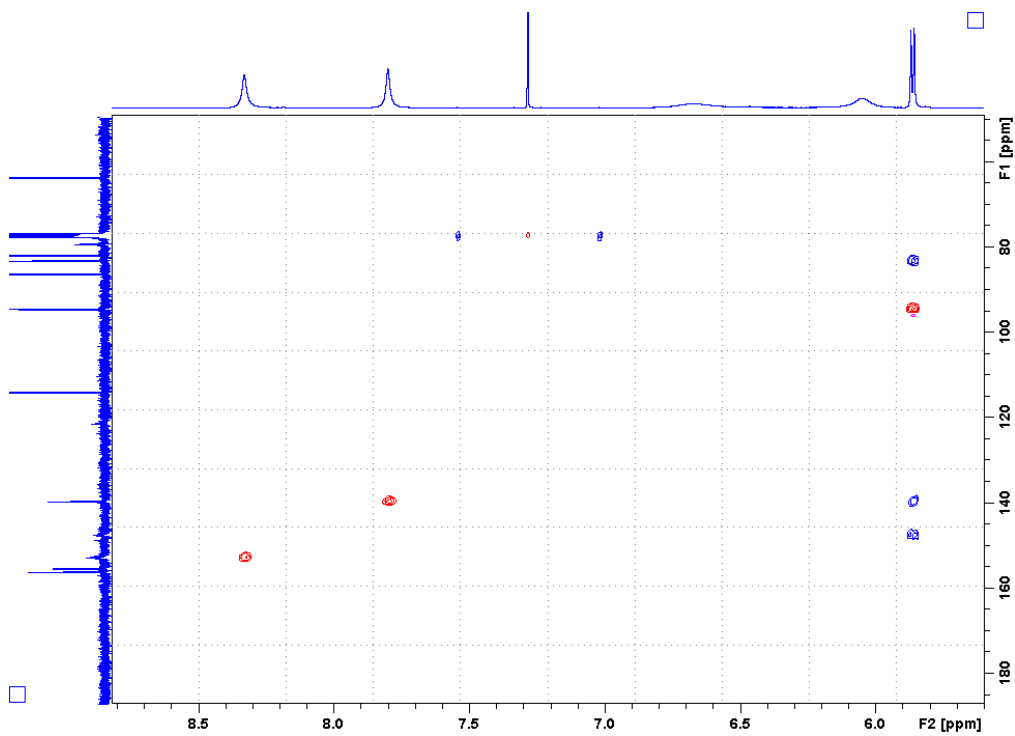
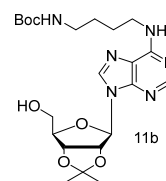
### *N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminoethyl-2',3'-*O*-isopropylidene-adenosine (**11a**).

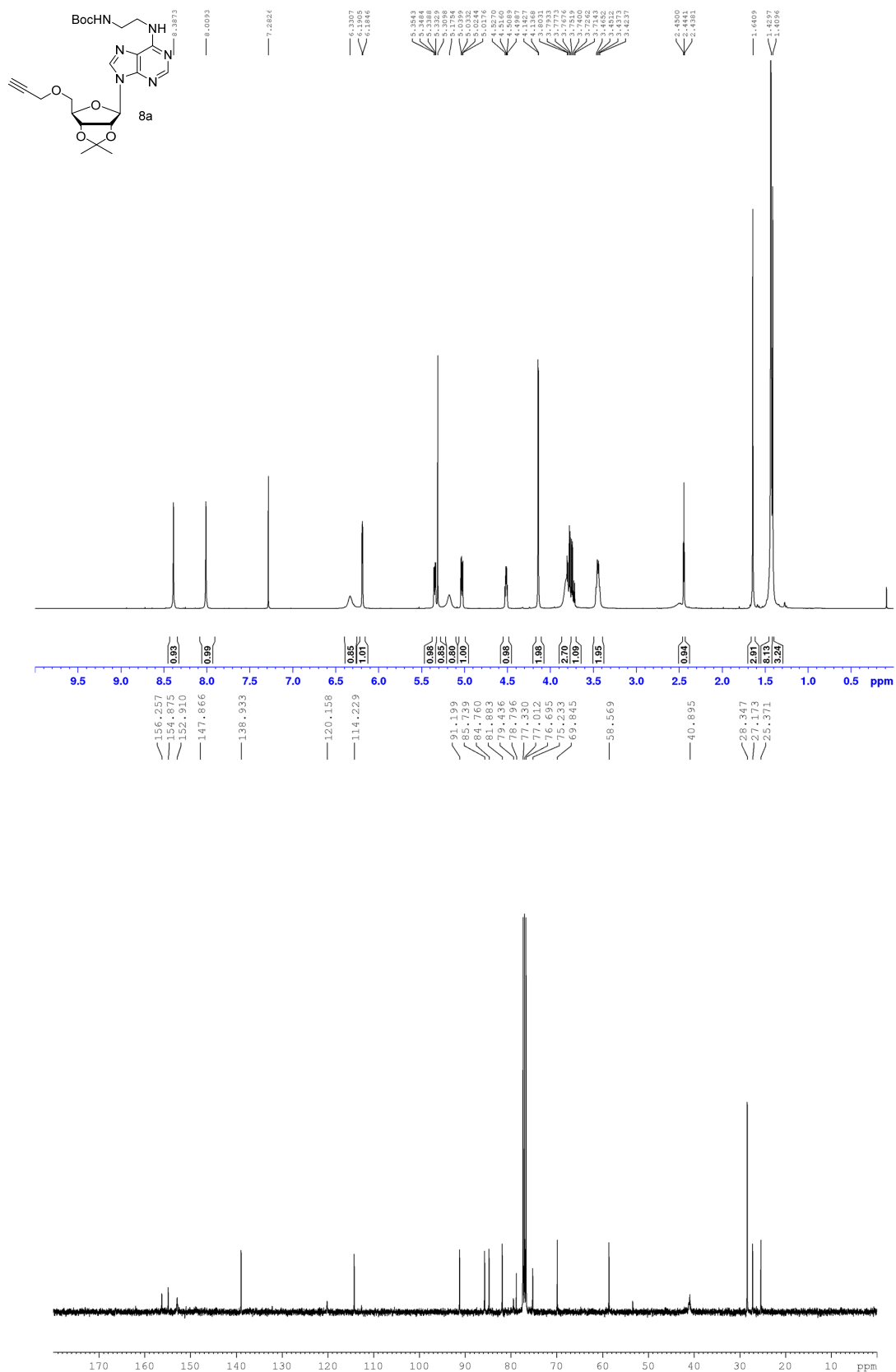


*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminoethyl-2',3'-*O*-isopropylidene-adenosine (**11a**).

*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminobutyl-2',3'-*O*-isopropylidene-adenosine (**11b**).

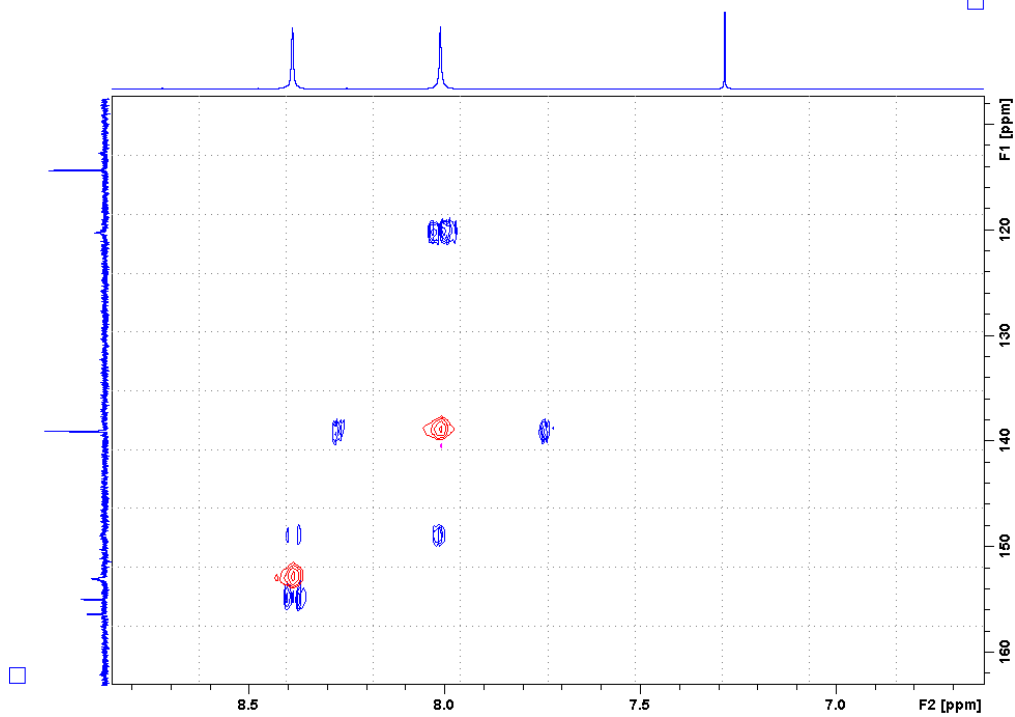
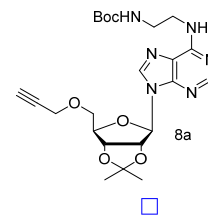
*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminobutyl-2',3'-*O*-isopropylidene-adenosine (**11b**).

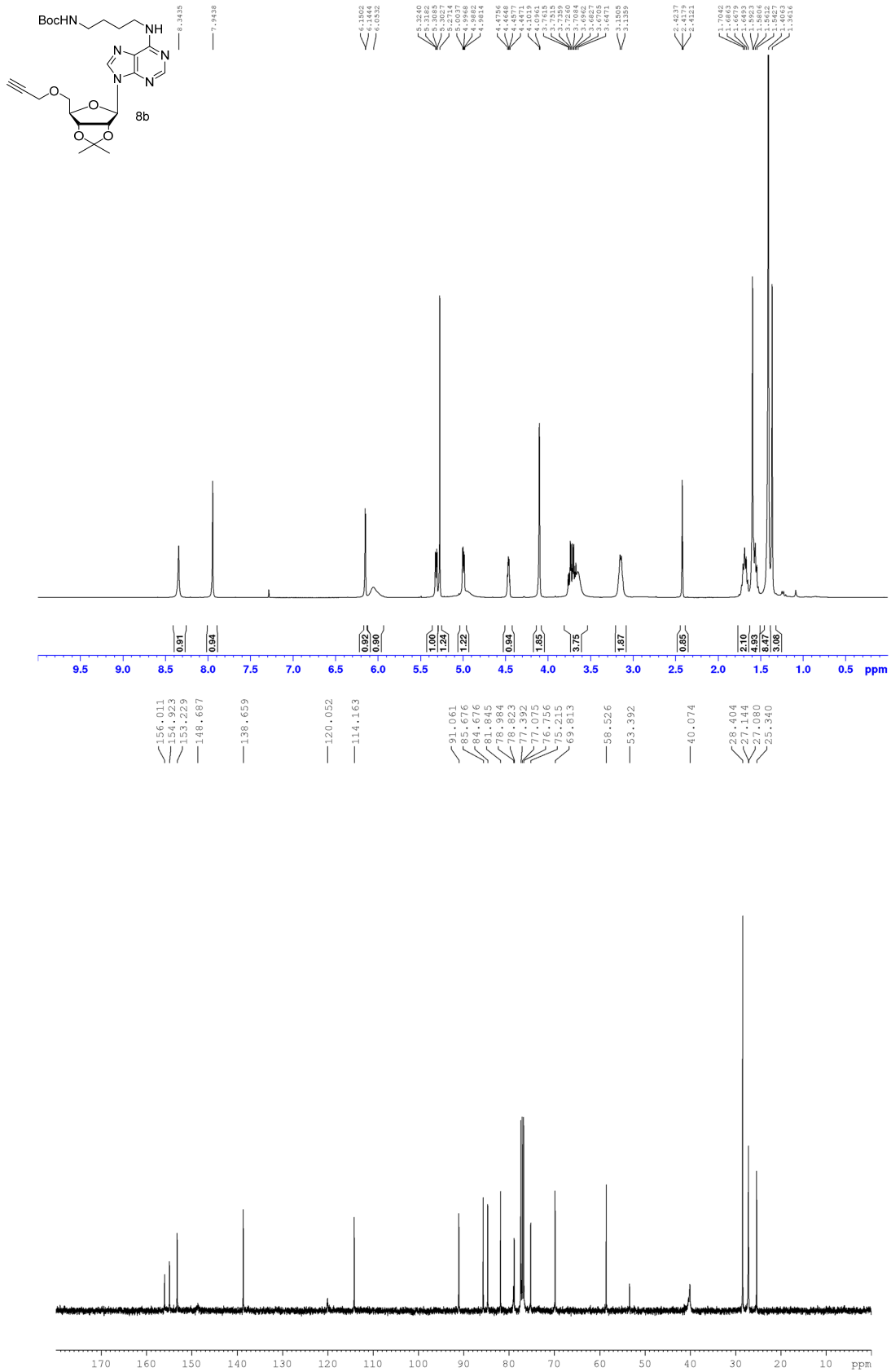


*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminoethyl-2',3'-*O*-isopropylidene-5'-*O*-propargyl-adenosine (**8a**).

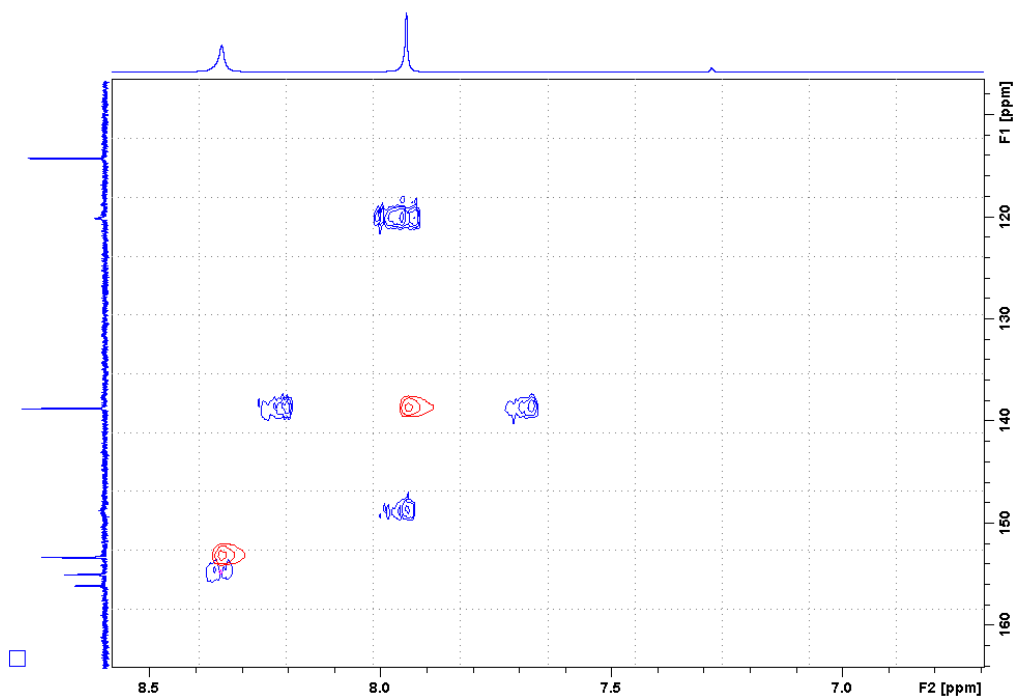
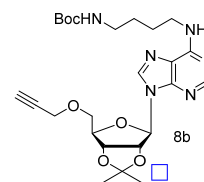


*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminoethyl-2',3'-*O*-isopropylidene-5'-*O*-propargyl-adenosine (**8a**).

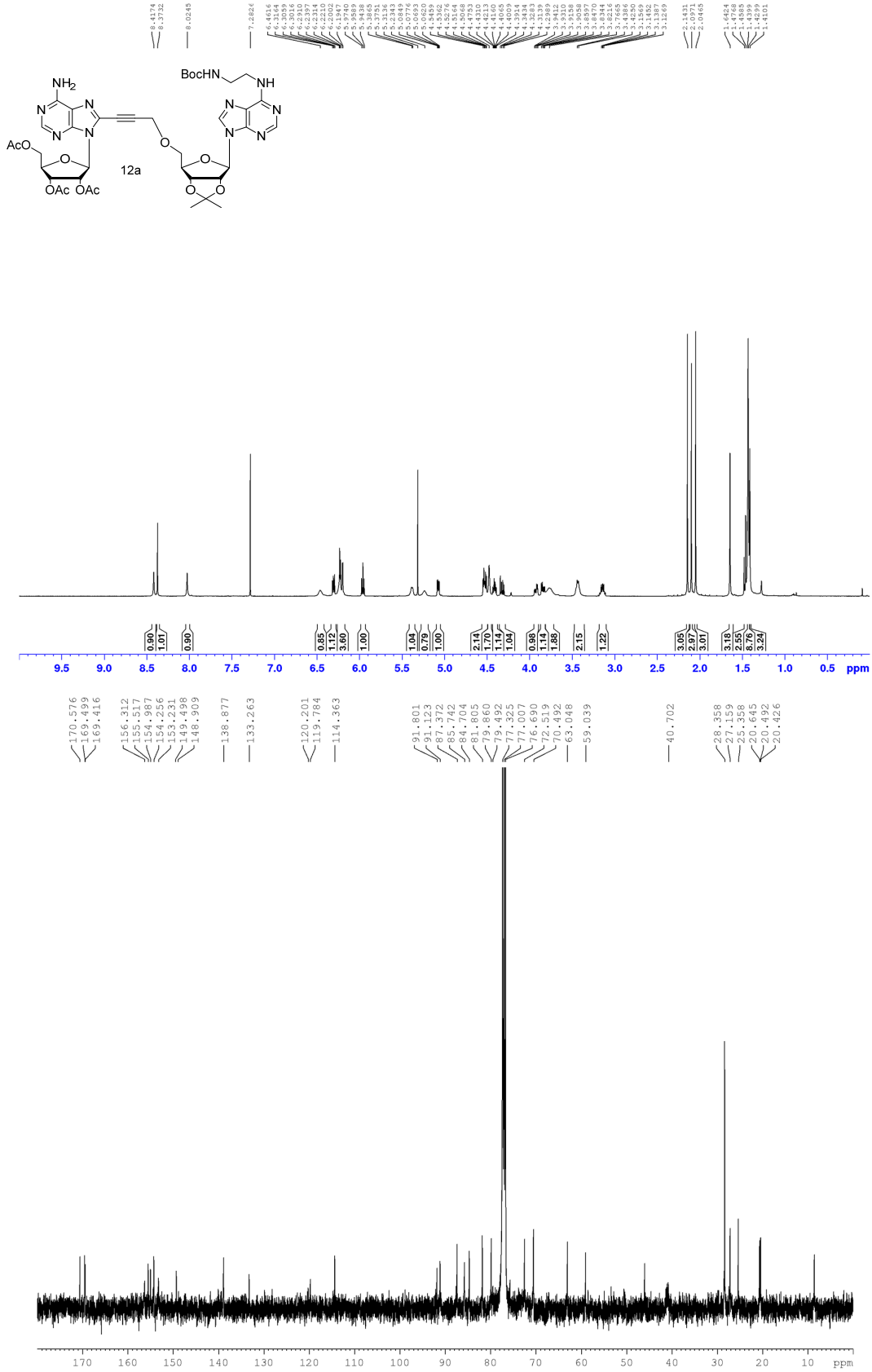


*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminobutyl-2',3'-*O*-isopropylidene-5'-*O*-propargyl-adenosine (**8b**).

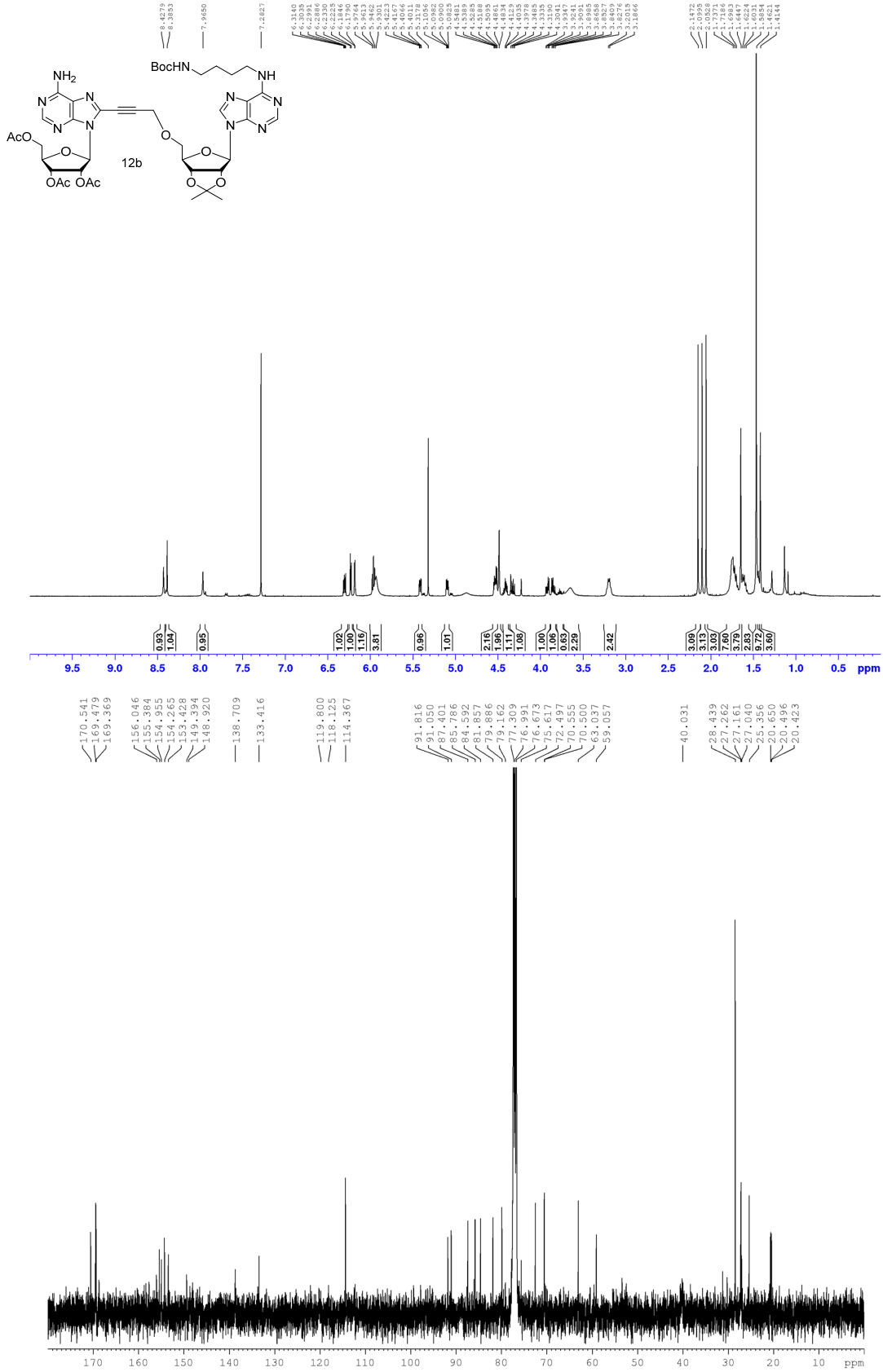
*N*<sup>6</sup>-(2-*tert*-Butyloxycarbonyl)aminobutyl-2',3'-*O*-isopropylidene-5'-*O*-propargyl-adenosine (**8b**).

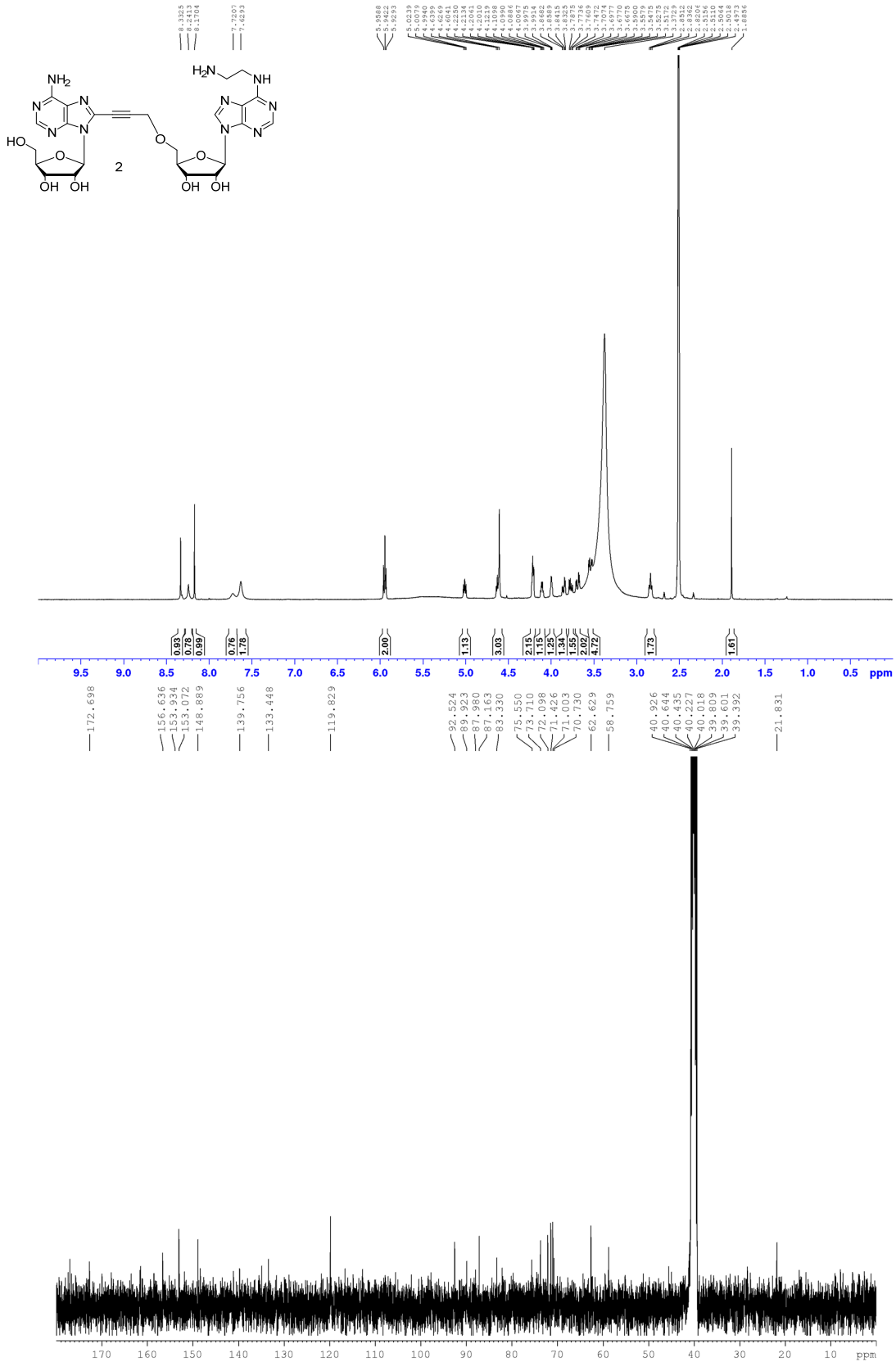


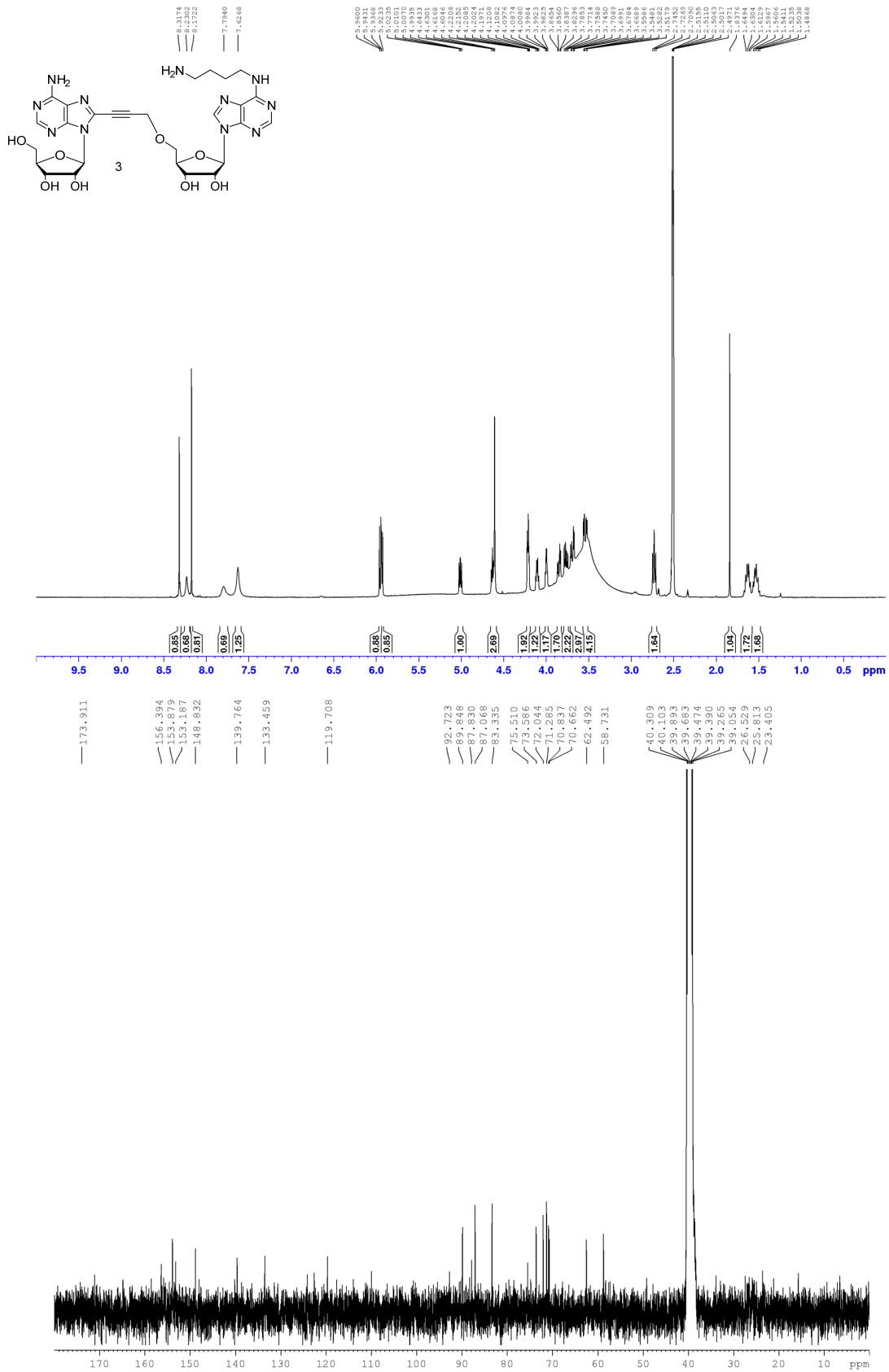
2',3',5'-Tri-*O*-acetyl-8-[3-(*N*<sup>6</sup>-(2-*tert*-butyloxycarbonyl)aminoethyl-2',3'-*O*-isopropylidene-5'-*O*-adenosinyl)propargyl]adenosine (**12a**).

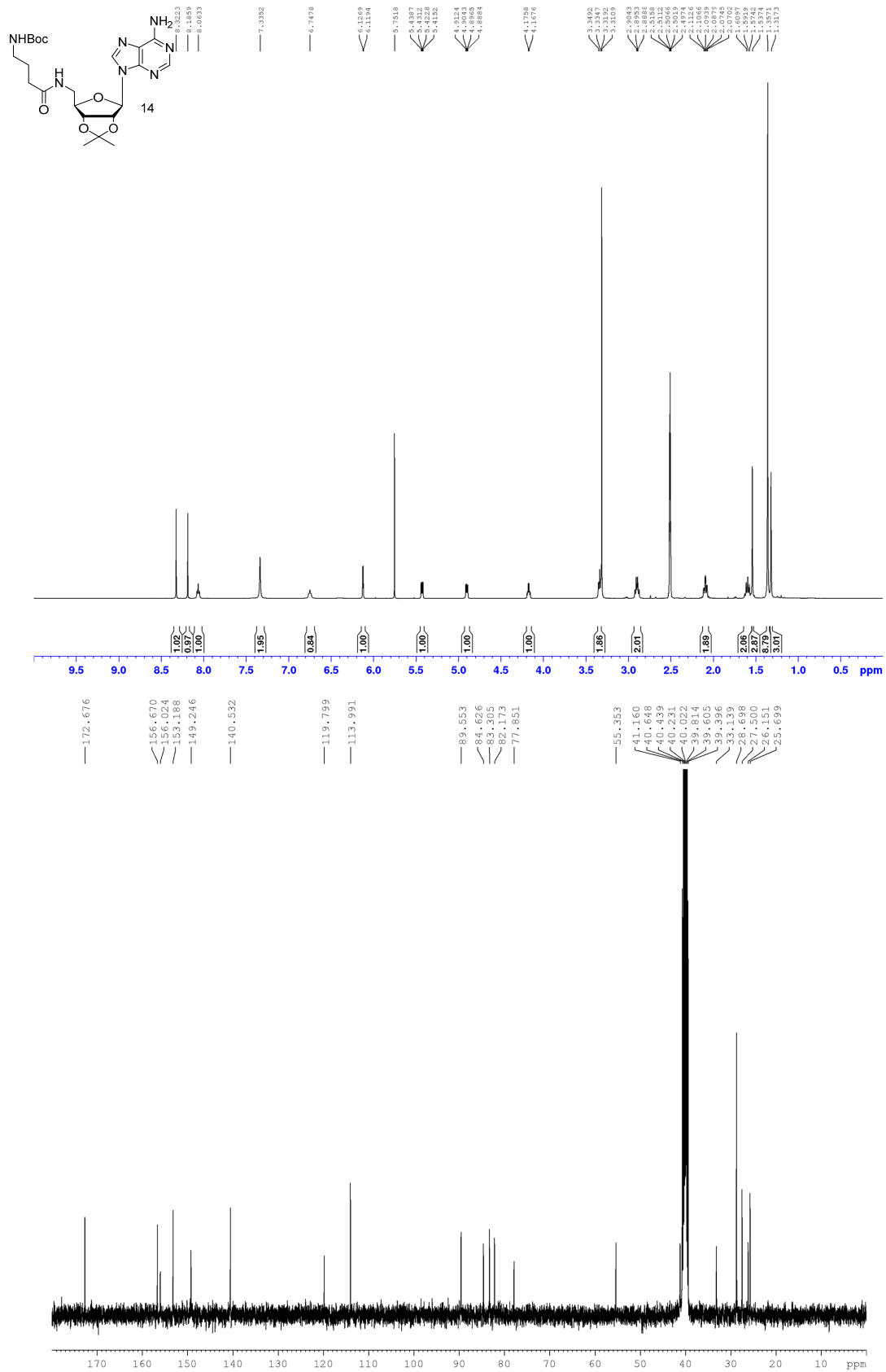


2',3',5'-Tri-*O*-acetyl-8-[3-(*N*<sup>6</sup>-(4-*tert*-butyloxycarbonyl)aminobutyl-2',3'-*O*-isopropylidene-5'-*O*-adenosinyl)propargyl]adenosine (**12b**).

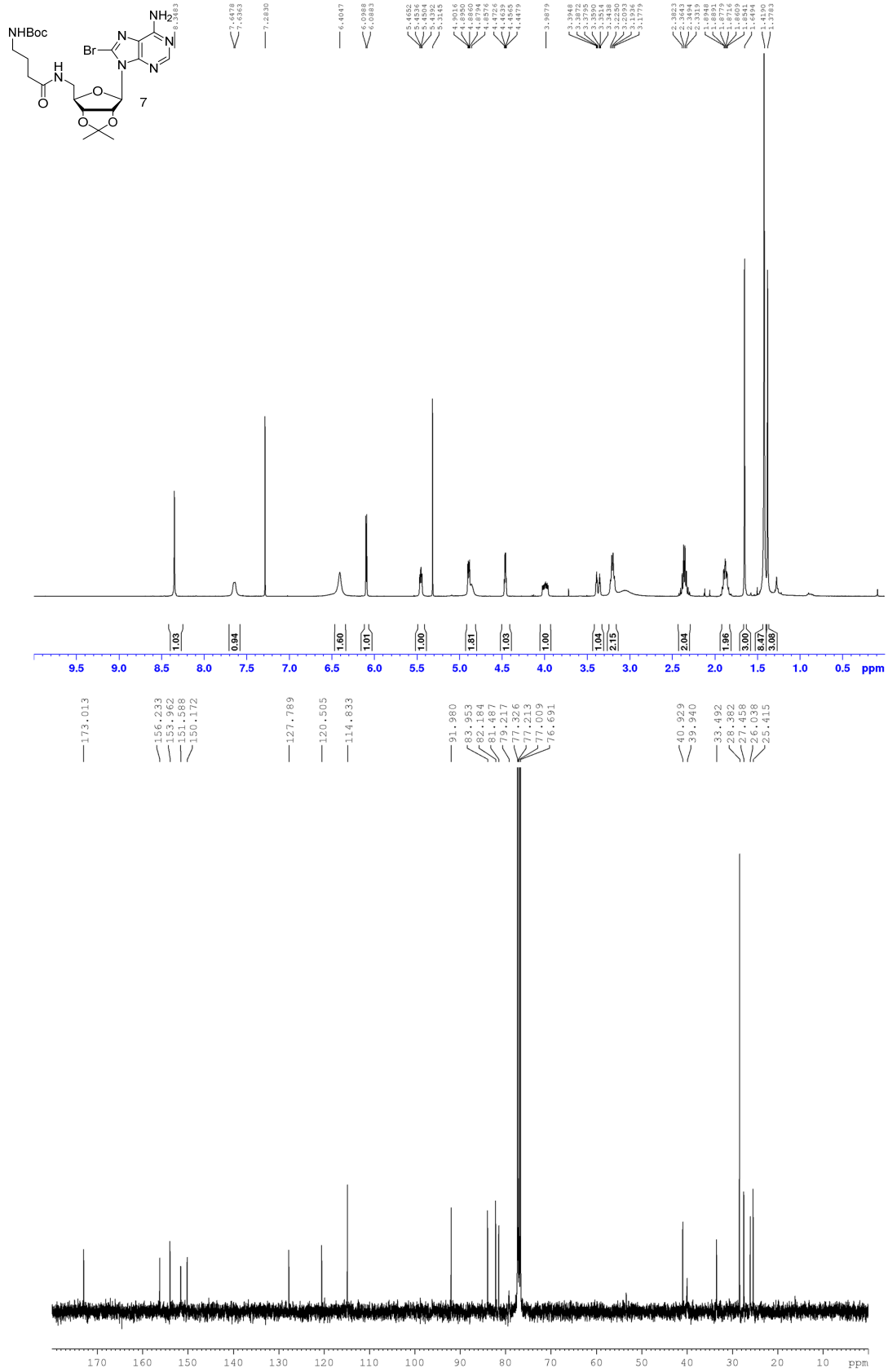


8-[3-(N<sup>6</sup>-2-Aminoethyl-5'-O-adenosinyl)propargyl]adenosine (2).

8-[3-(N<sup>6</sup>-4-Aminobutyl-5'-O-adenosinyl)propargyl]adenosine (3).

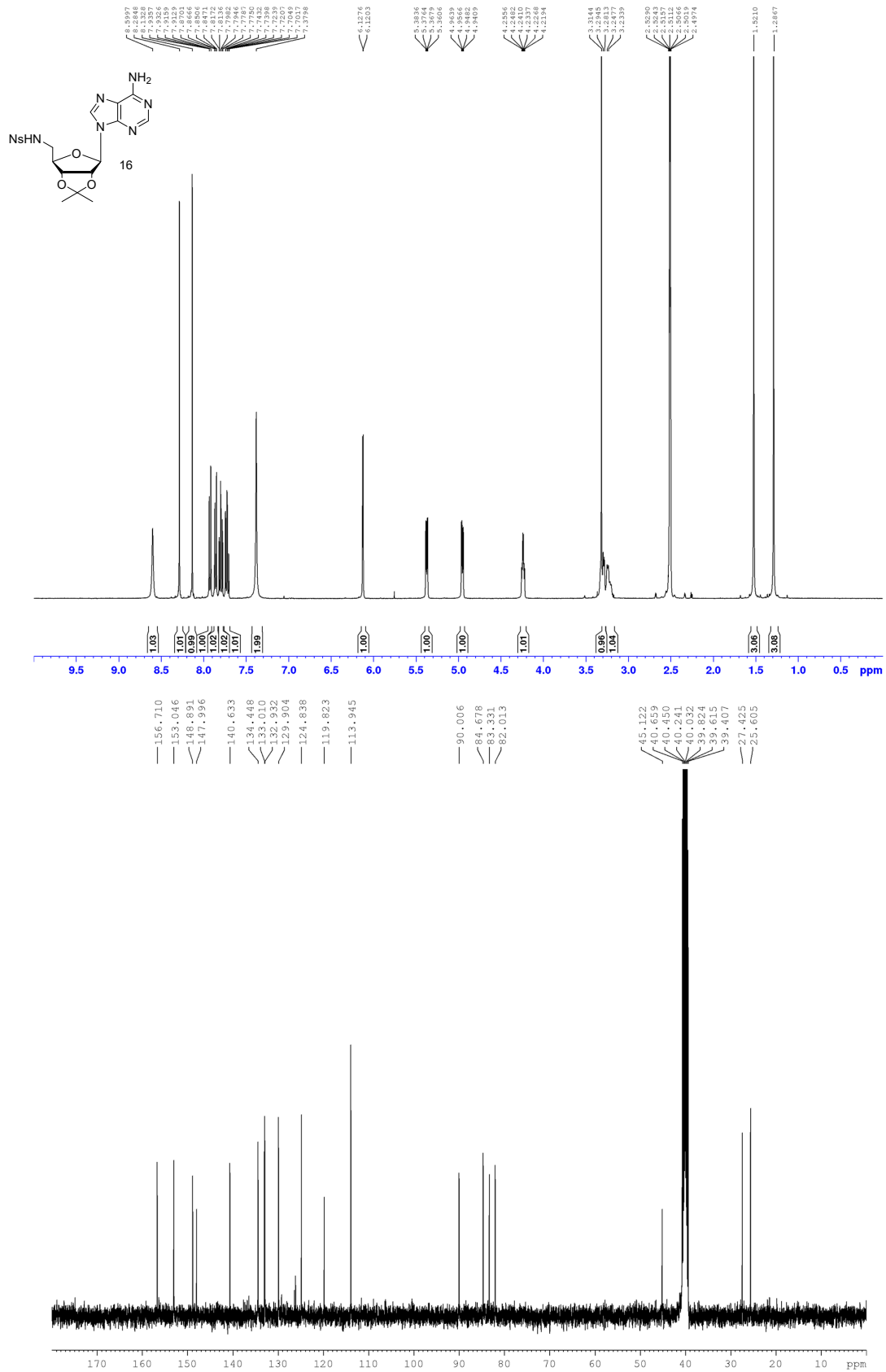
5'-[4-(*N*-*tert*-Butyloxycarbonyl-amino)butylamido]-5'-deoxy-2',3'-*O*-isopropylidene-adenosine (14).



8-Bromo-5'-(4-(*N*-*tert*-butyloxycarbonyl-amino)butylamido)-5'-deoxy-2',3'-*O*-isopropylidene-adenosine (7).





5'-Deoxy-5'-(2-nitrobenzenesulfonamido)-2',3'-O-isopropylidene-adenosine (**16**).



5'-N-(*N*-*tert*-Butyloxycarbonyl-aminopropyl)propargylamino-5'-deoxy-2',3'-*O*-isopropylidene-adenosine (**18**).