

# Supporting Information

for

## Substituent effect on the energy barrier for $\sigma$ -bond formation from $\pi$ -single-bonded species, singlet 2,2-dialkoxycyclopentane-1,3-diyls

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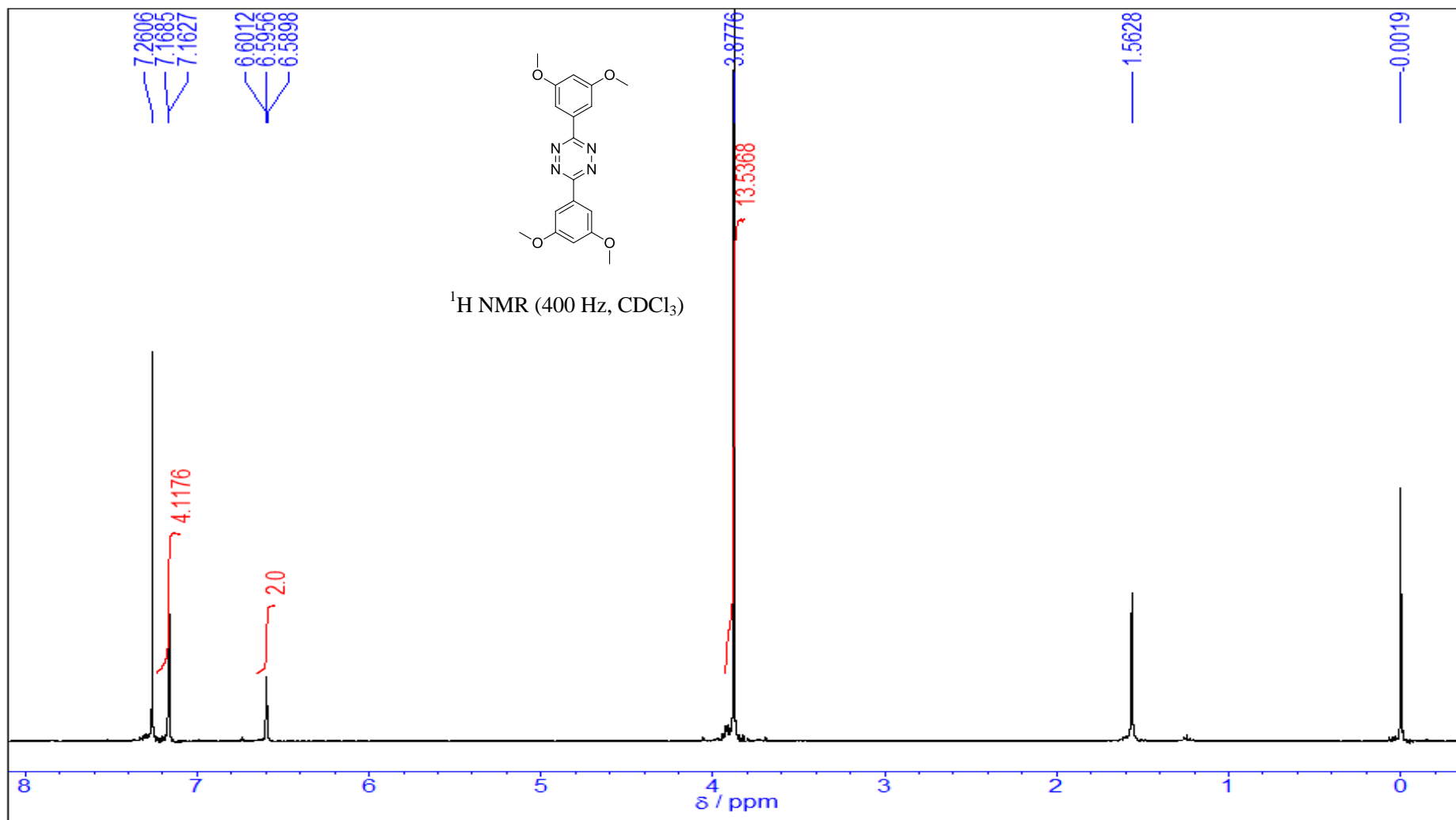
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Email: Manabu Abe - [mabe@hiroshima-u.ac.jp](mailto:mabe@hiroshima-u.ac.jp)

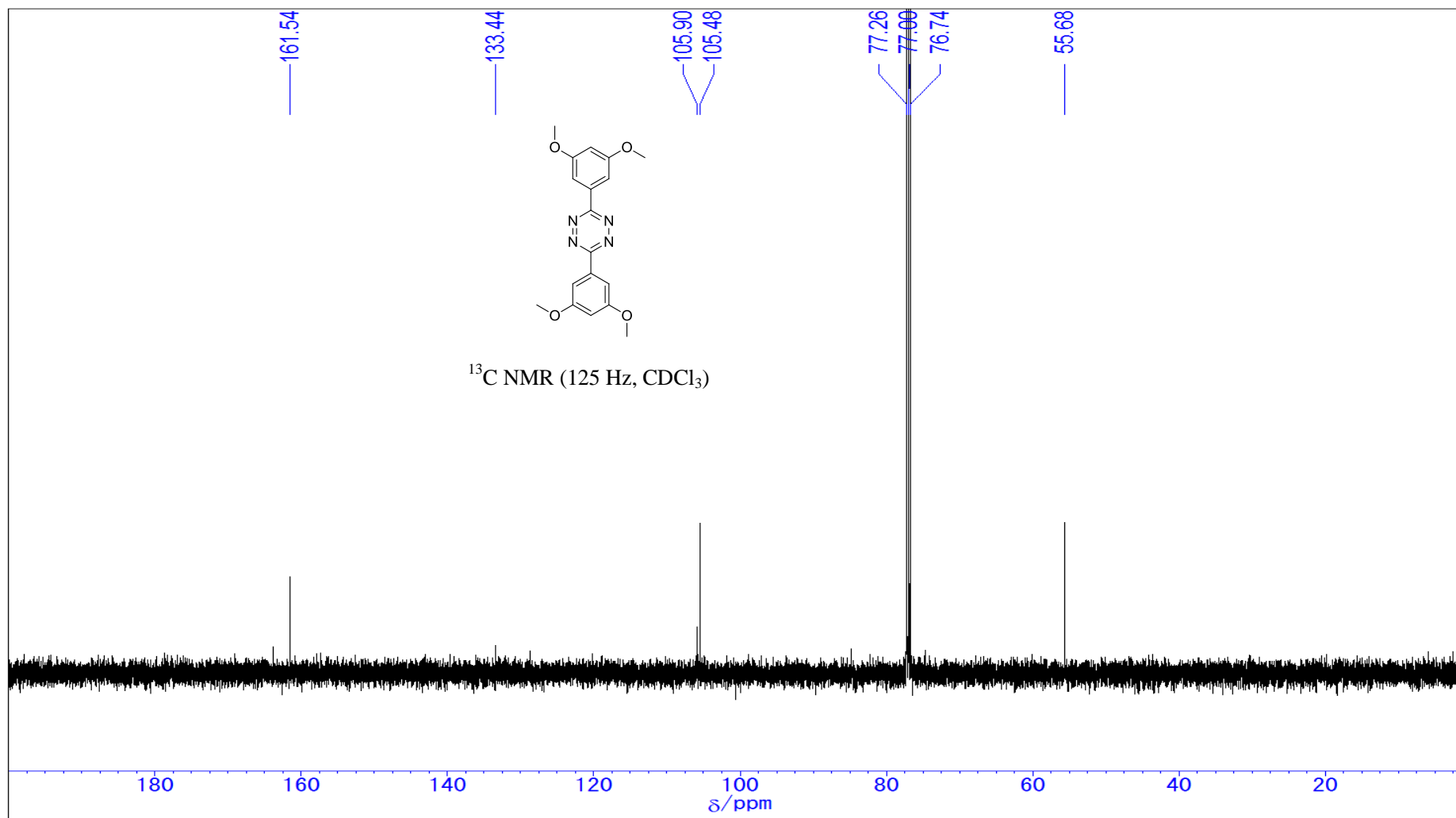
\* Corresponding author

NMR spectra of compounds **1–5**, **AZc–g**, and **CPc–g**

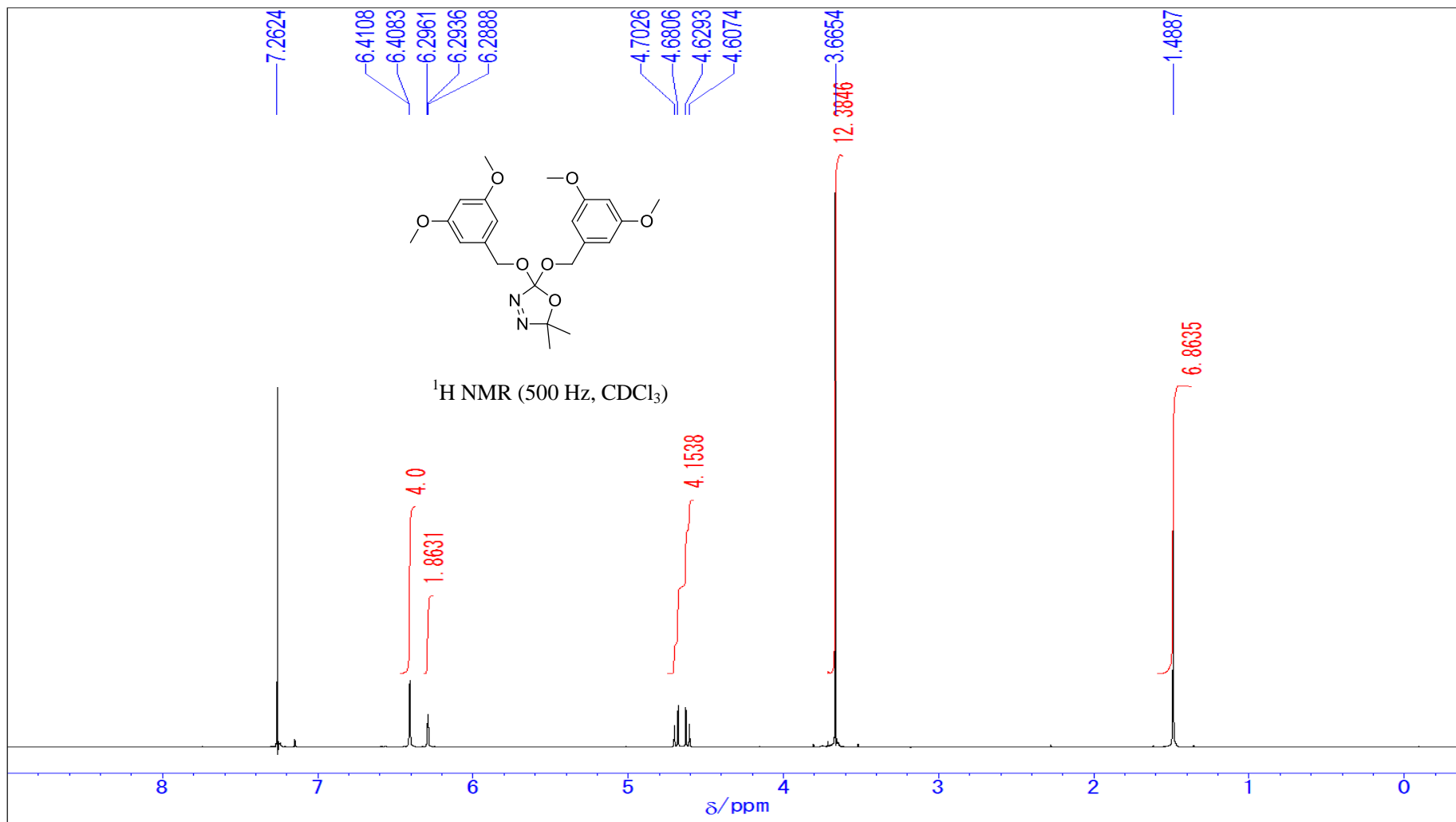
3,5-Dimethoxyphenyl-[1,2,4,5]tetrazine (1f)  $^1\text{H}$  NMR



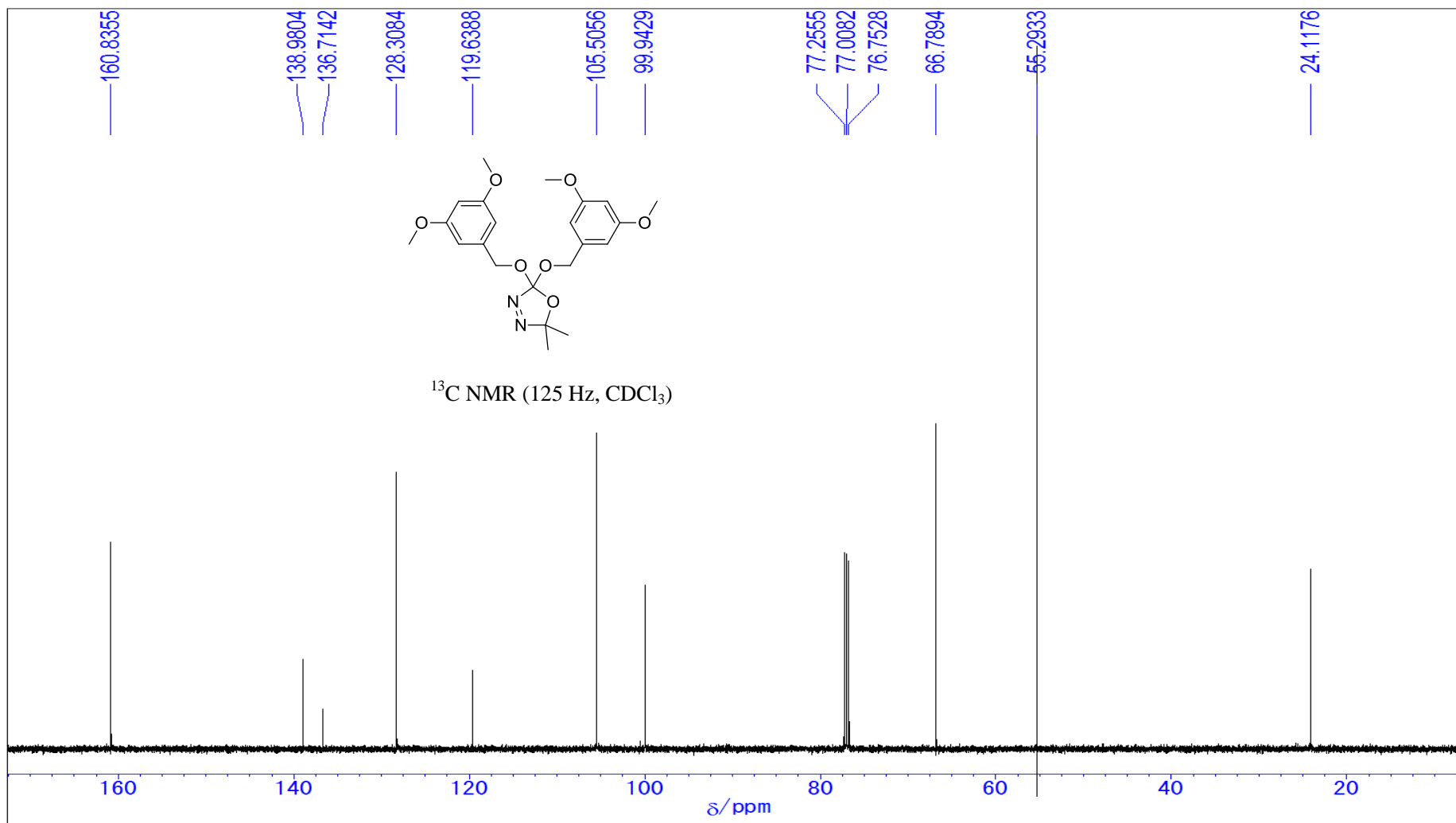
3,5-Dimethoxyphenyl-[1,2,4,5]tetrazine (1f)  $^{13}\text{C}$  NMR



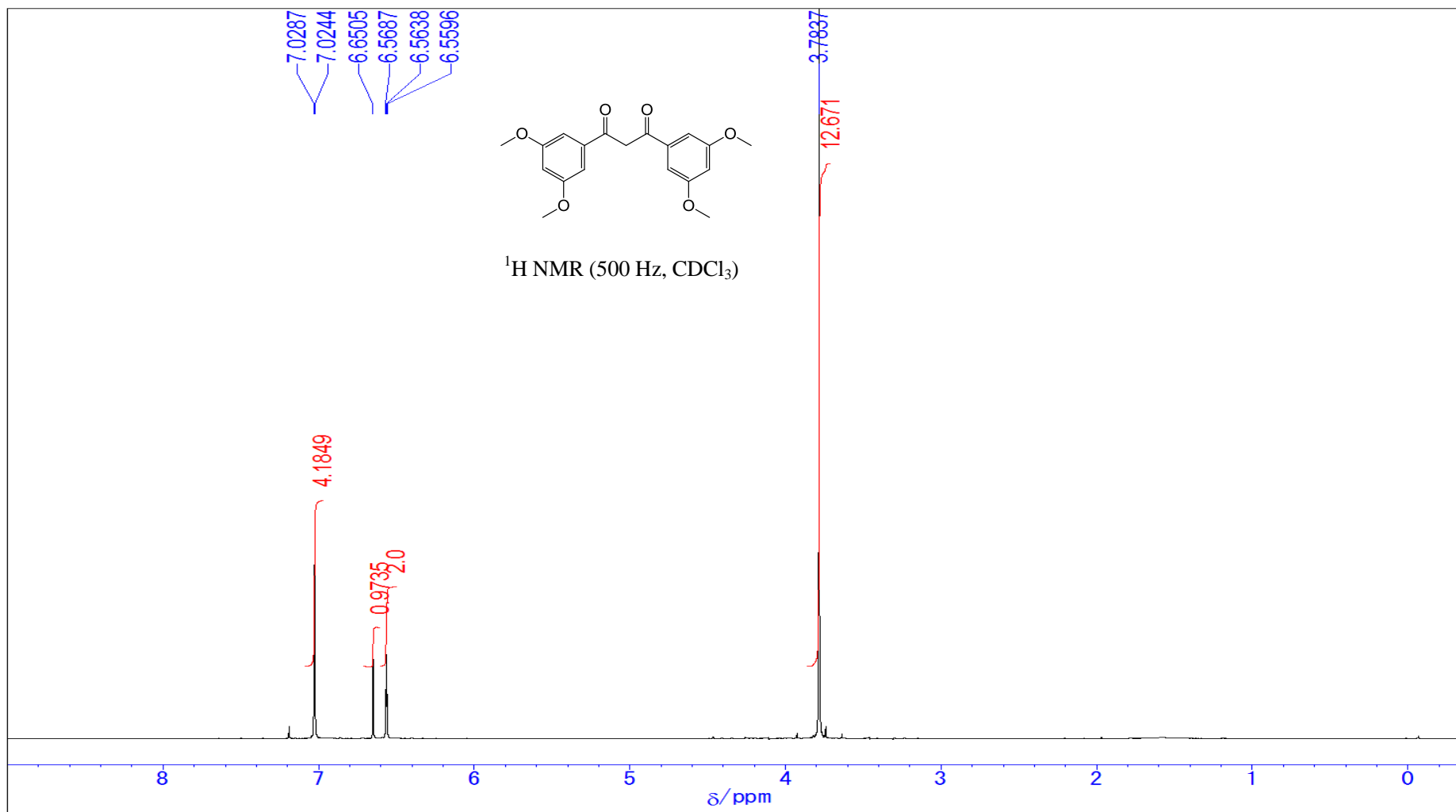
5,5-Dimethyl-2,2-bis(3,5-dimethoxybenzyl)- $\Delta^3$ -1,3,4-oxadiazoline (2f)  $^1\text{H}$  NMR



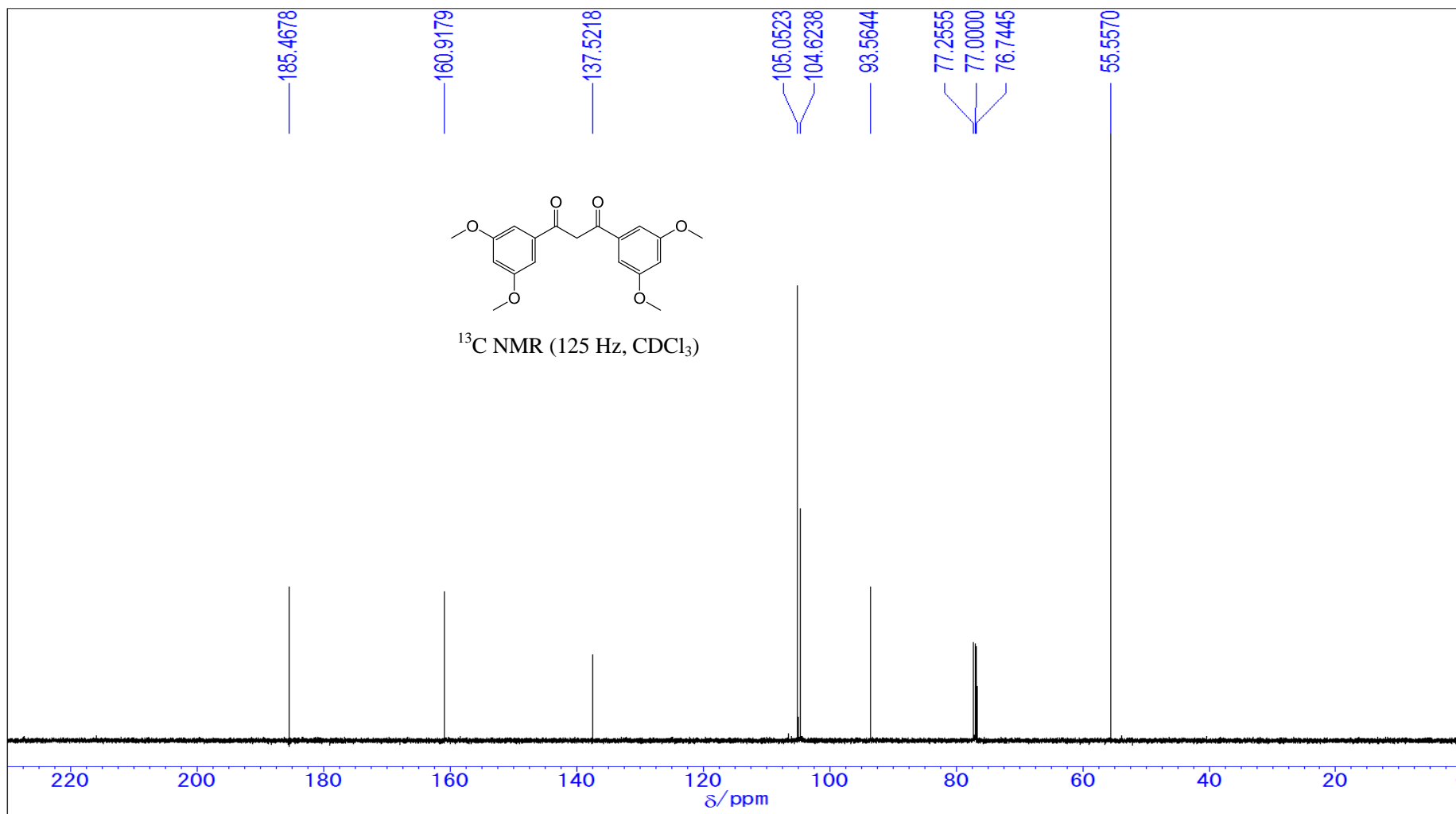
5,5-Dimethyl-2,2-bis(3,5-dimethoxybenzyl)- $\Delta^3$ -1,3,4-oxadiazoline (2f)  $^{13}\text{C}$  NMR



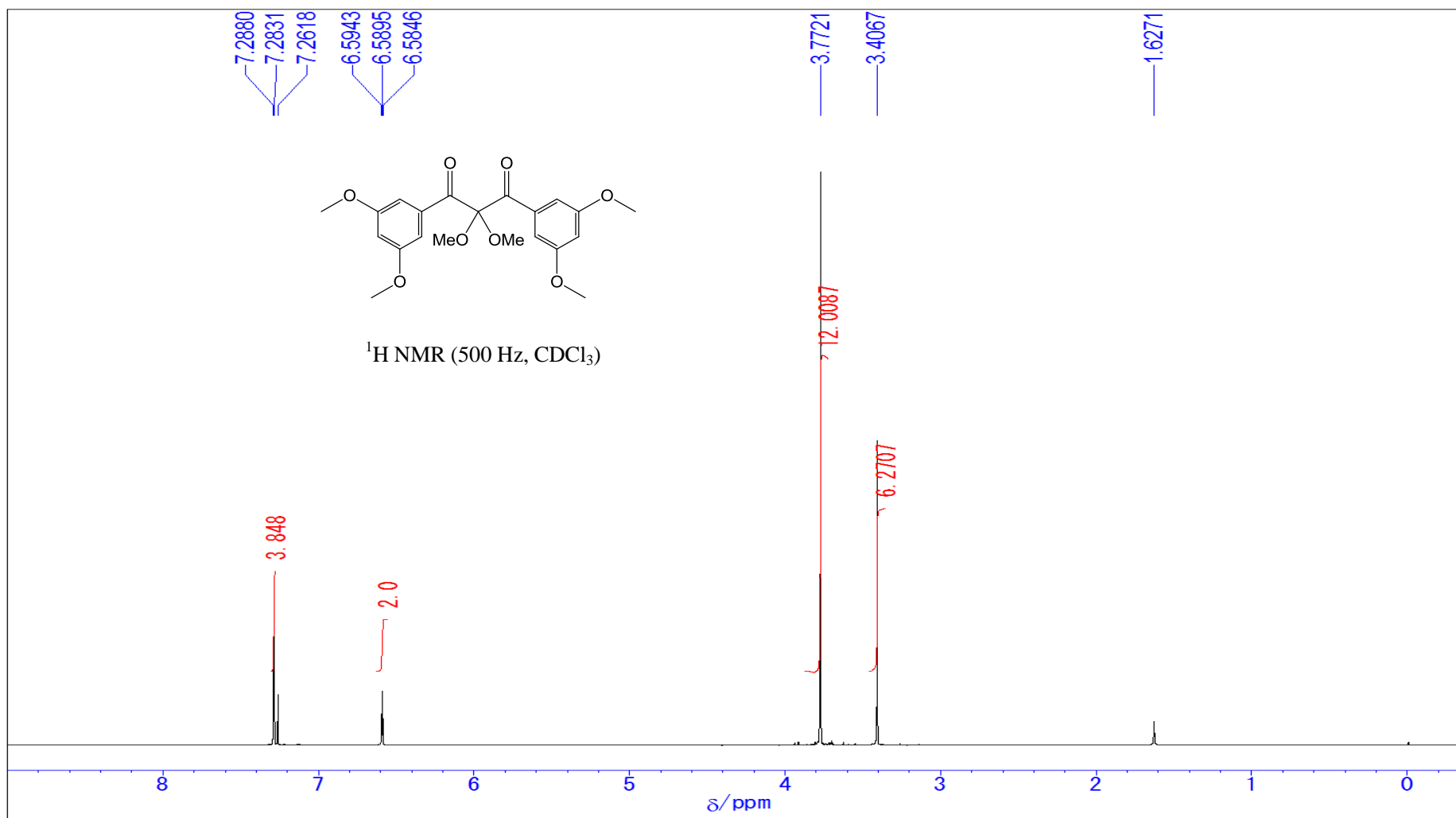
1,3-Bis(3,5-dimethoxyphenyl)propane-1,3-dione (4)  $^1\text{H}$  NMR



1,3-Bis(3,5-dimethoxyphenyl)propane-1,3-dione (4) <sup>1</sup>H NMR

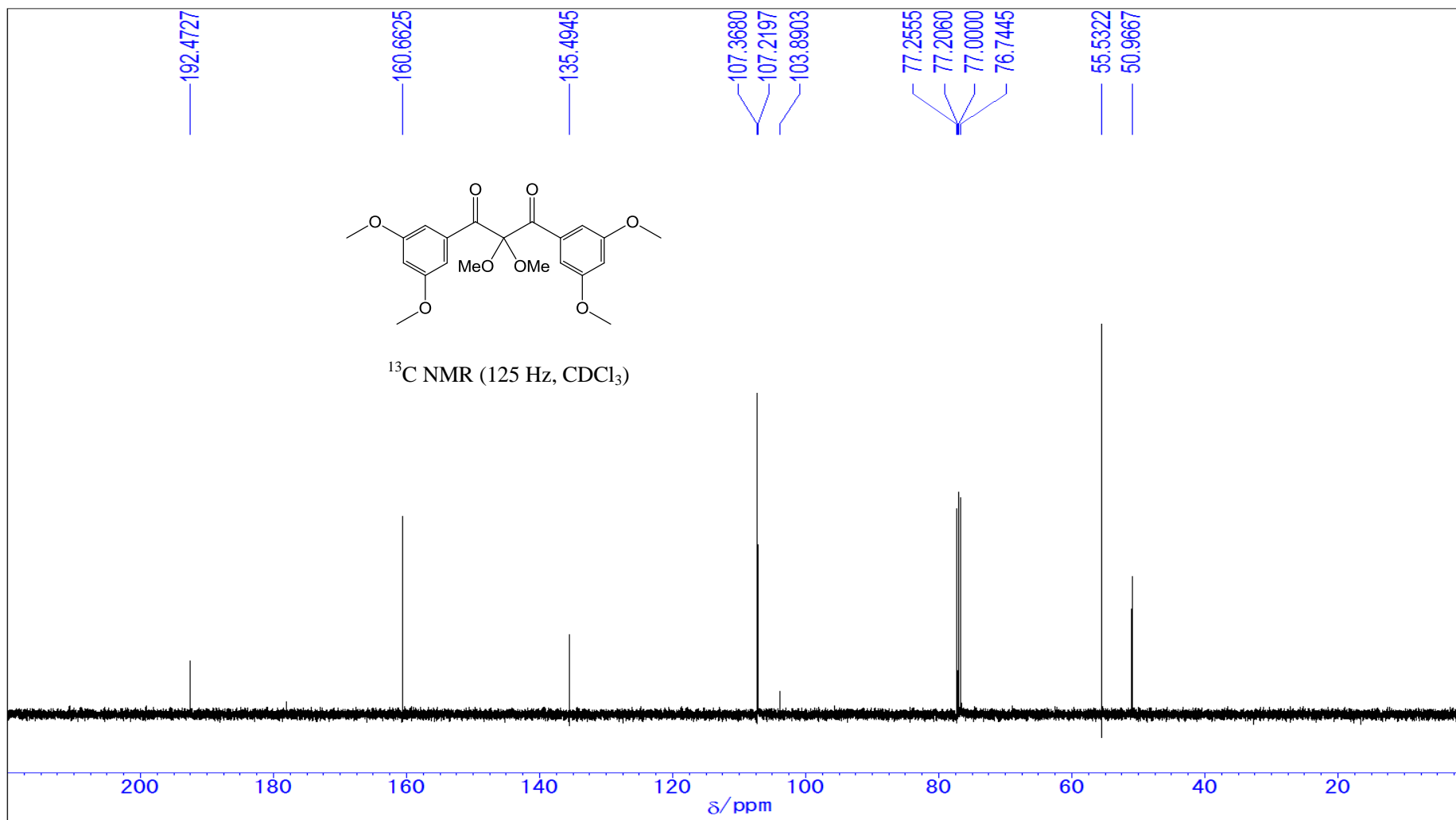


1,3-Bis(3,5-dimethoxyphenyl)-2,2-dimethoxypropane-1,3-dione (5)  $^{13}\text{C}$  NMR

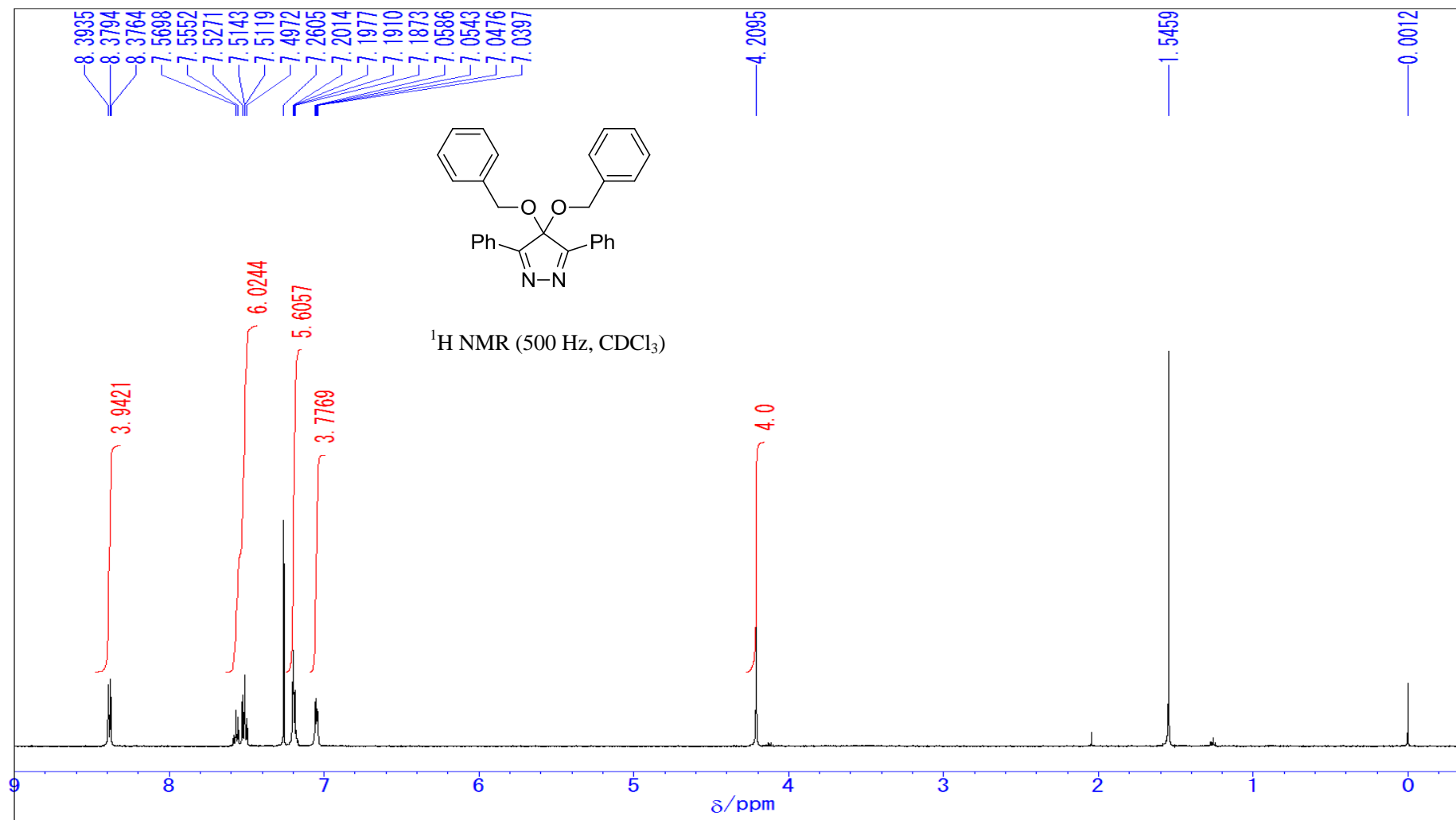




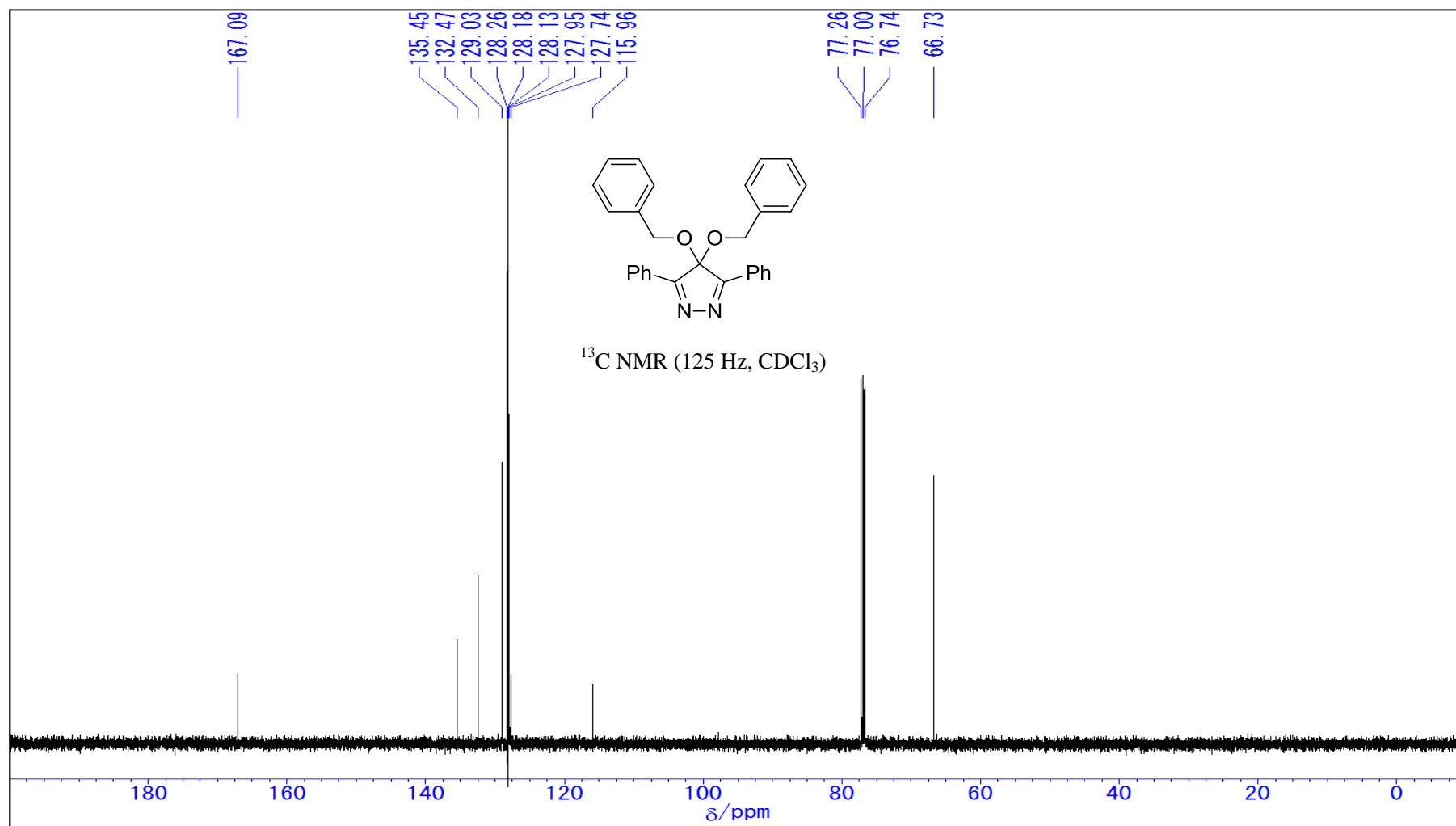
1,3-Bis(3,5-dimethoxyphenyl)-2,2-dimethoxypropane-1,3-dione (5) <sup>13</sup>C NMR



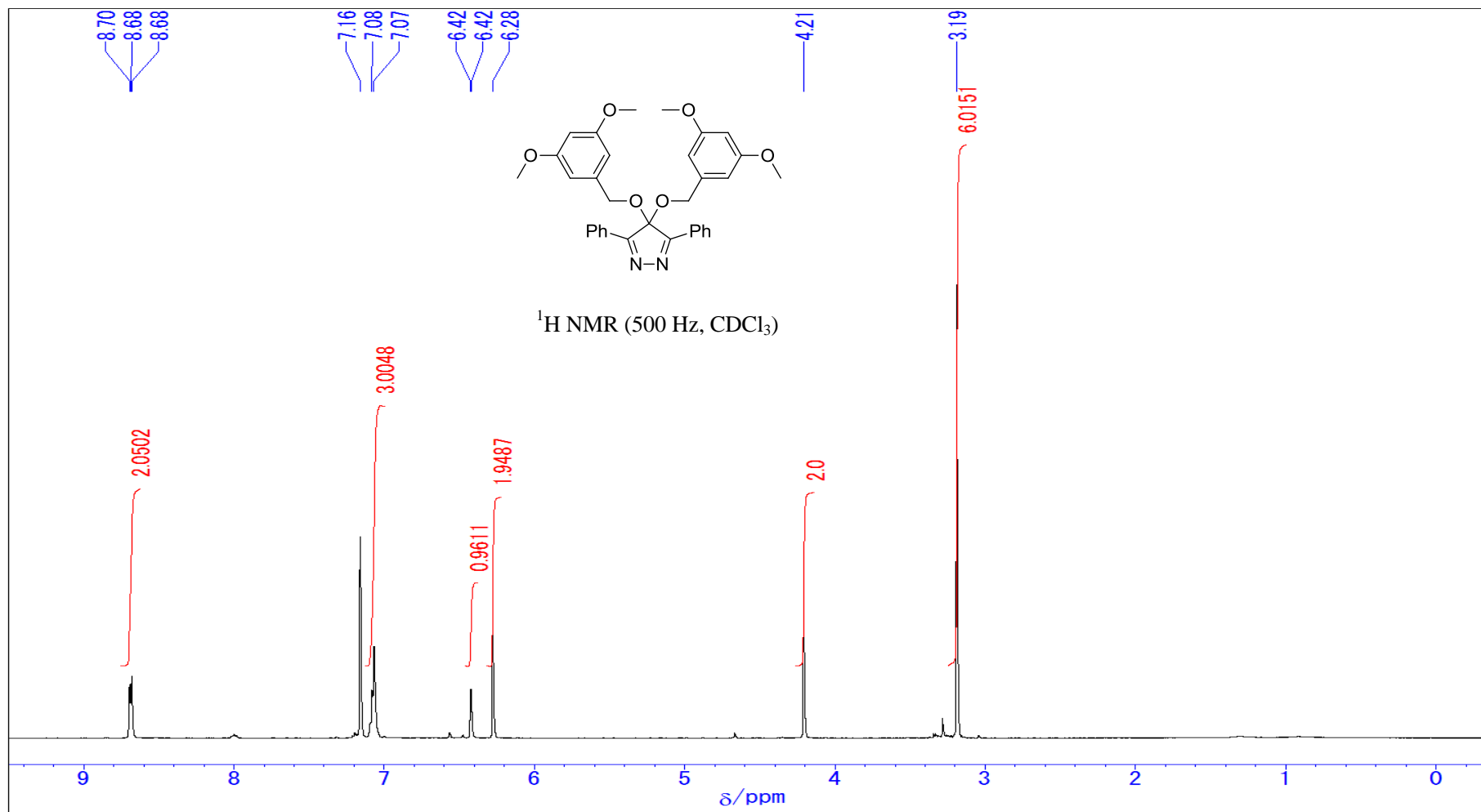
### 4,4-Dibenzyloxy-3,5-diphenylpyrazole (3c) <sup>1</sup>H NMR



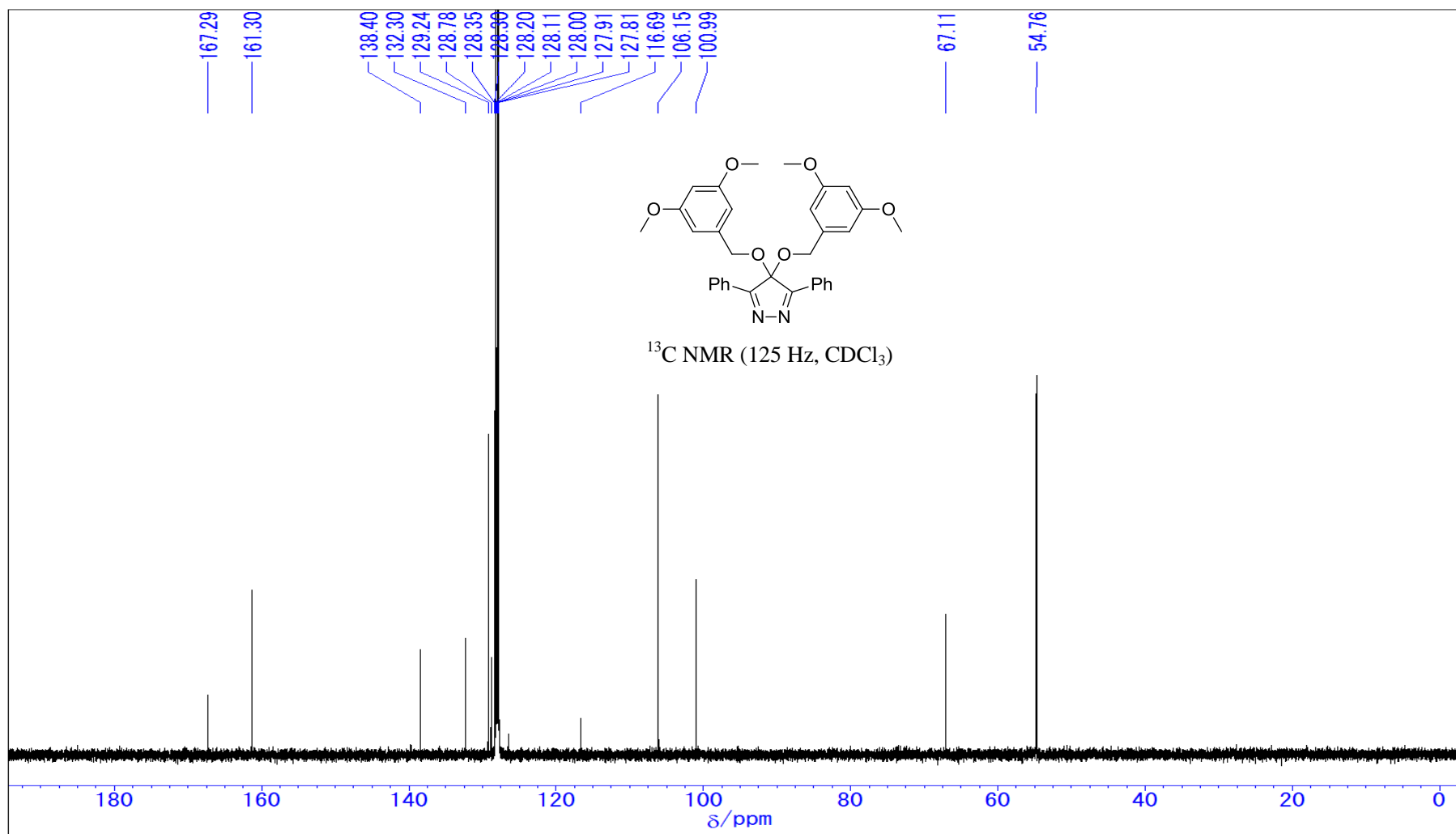
4,4-Dibenzyloxy-3,5-diphenylpyrazole (3c)  $^{13}\text{C}$  NMR



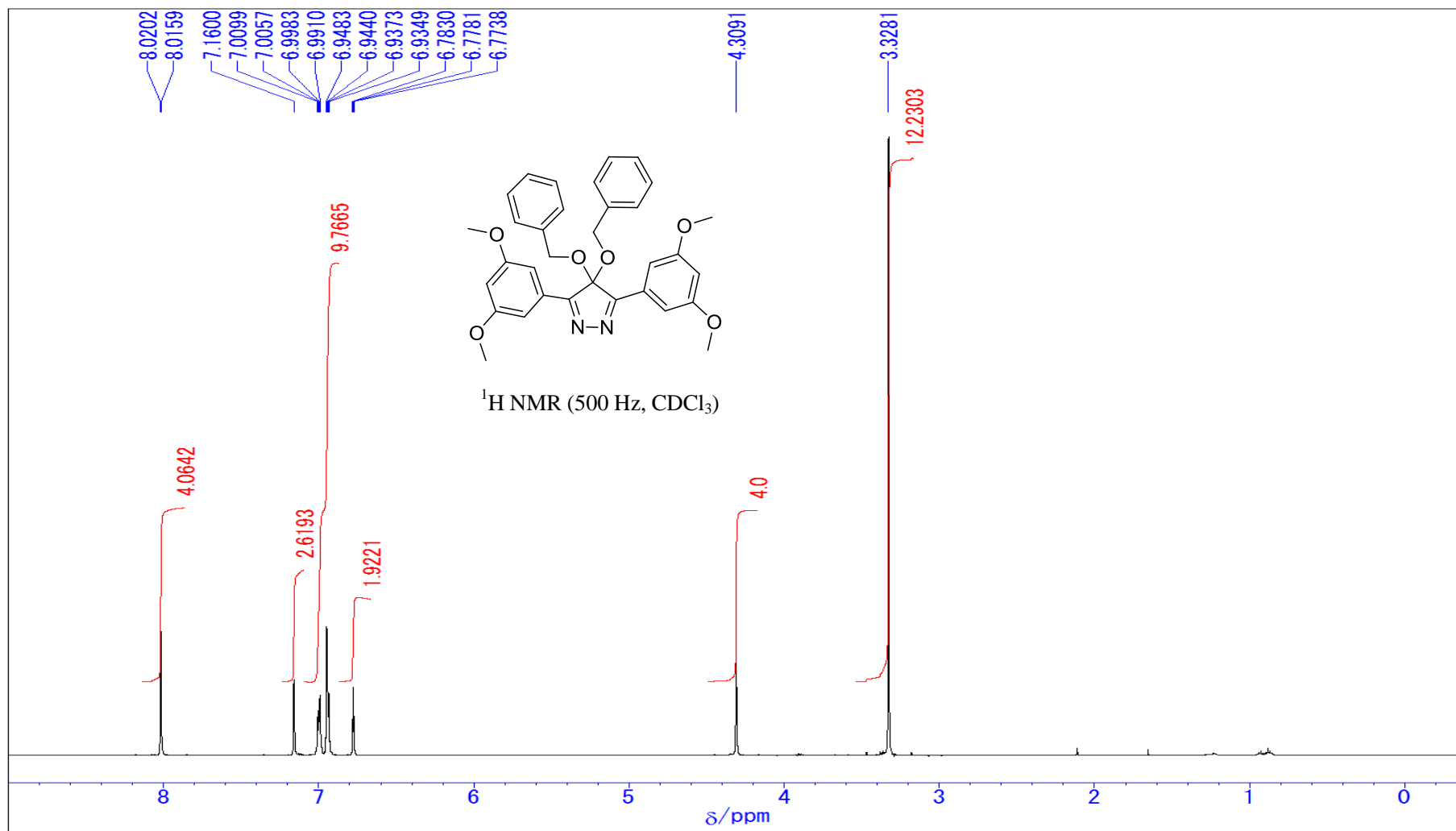
4,4-Bis(3,5-dimethoxybenzyloxy)-3,5-diphenylpyrazole (3d)  $^1\text{H}$  NMR



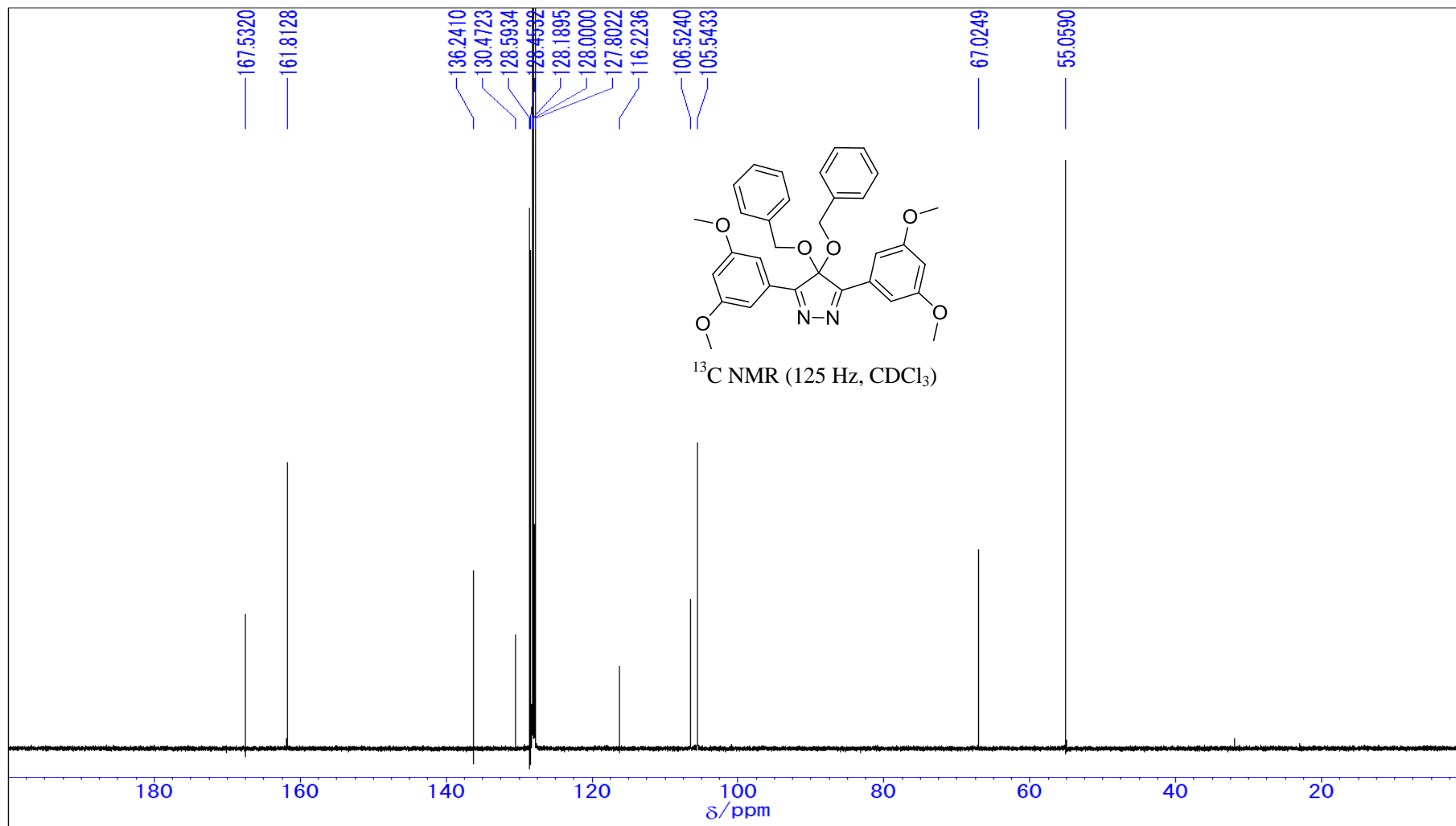
4,4-Bis(3,5-dimethoxybenzyloxy)-3,5-diphenylpyrazole (3d)  $^{13}\text{C}$  NMR



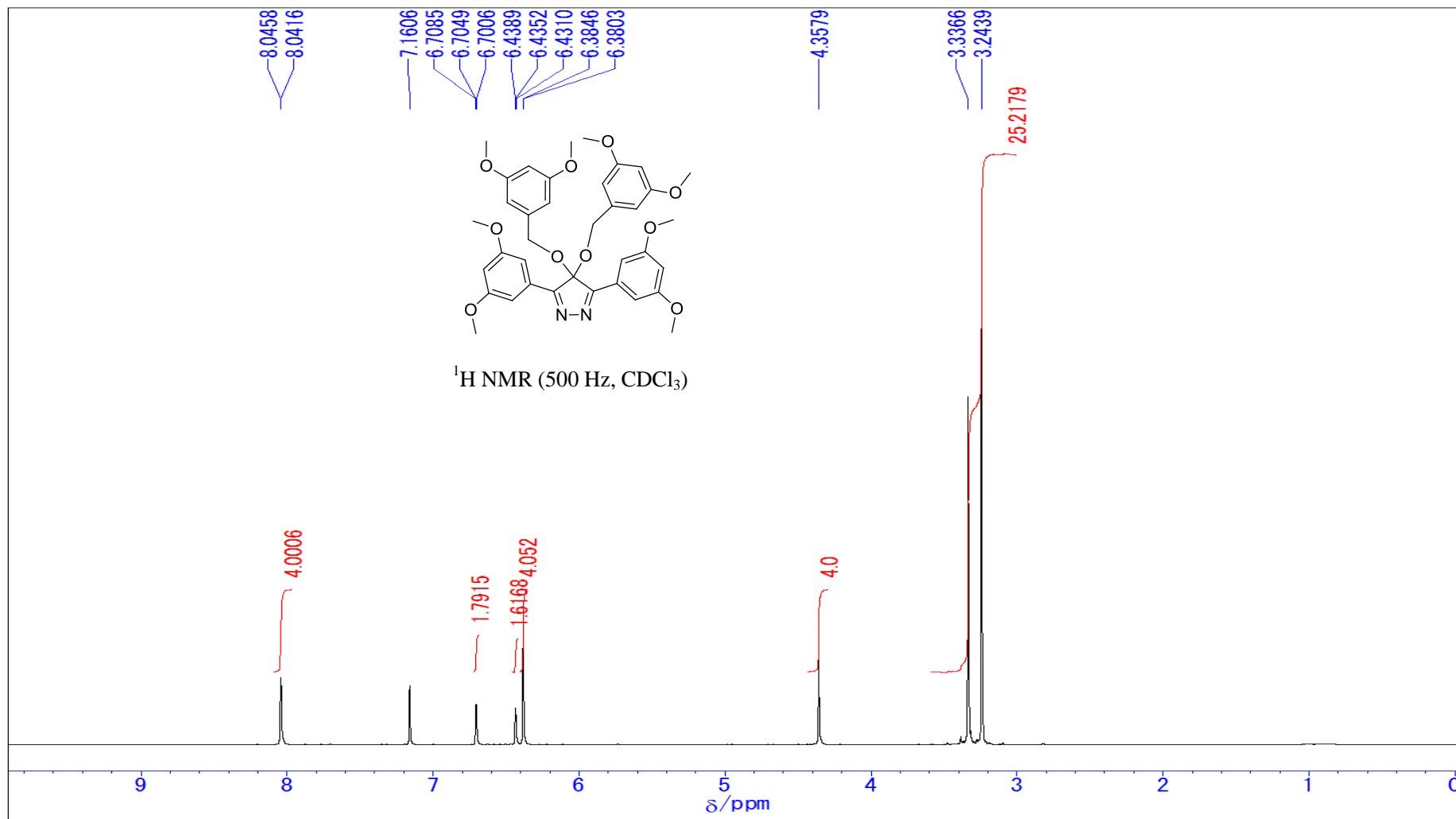
4,4-Dibenzyloxy-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3e)  $^1\text{H}$  NMR



4,4-Dibenzyloxy-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3e)  $^{13}\text{C}$  NMR

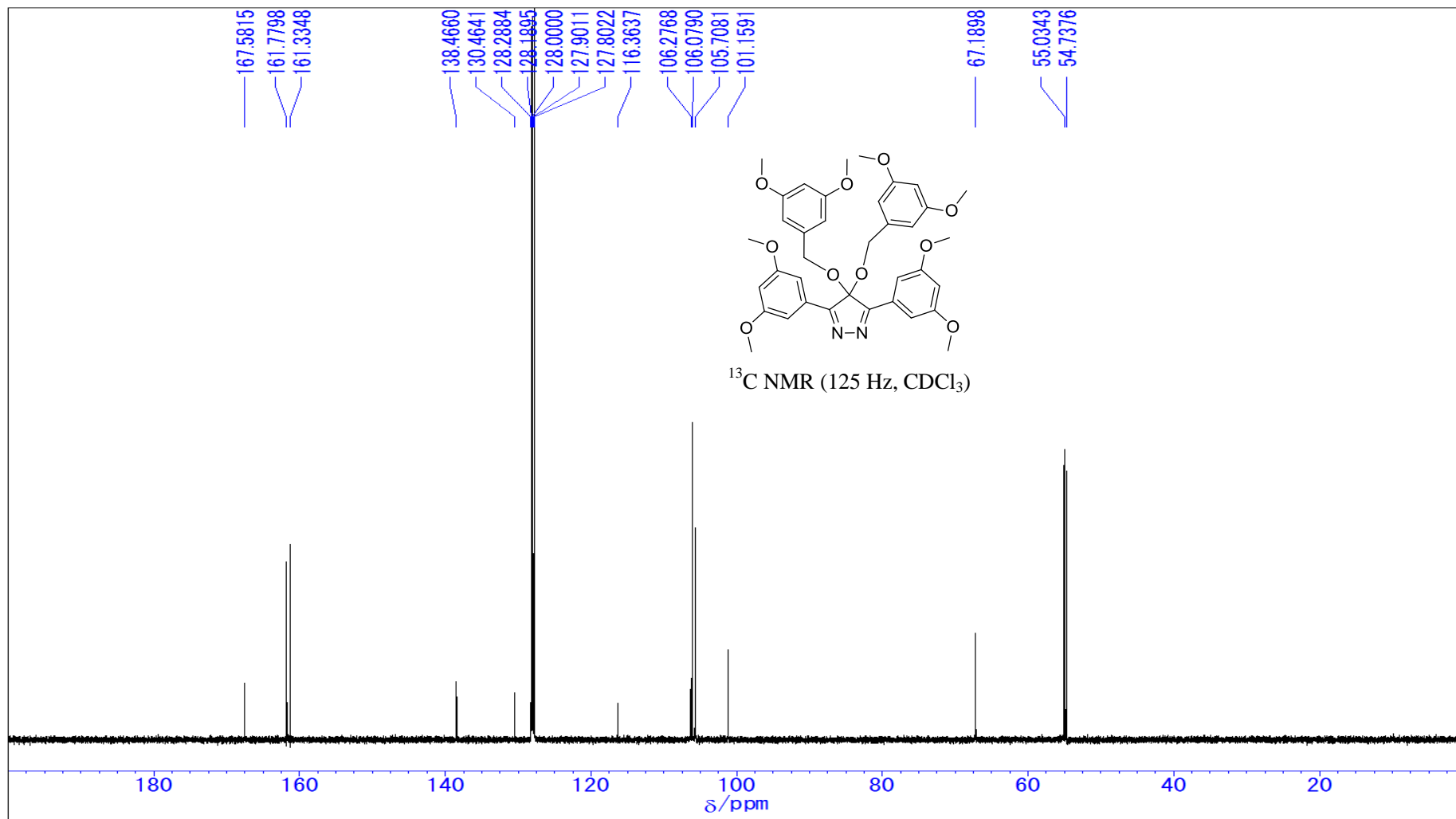


4,4-Bis(3,5-dimethoxybenzyloxy)-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3f) <sup>1</sup>H NMR

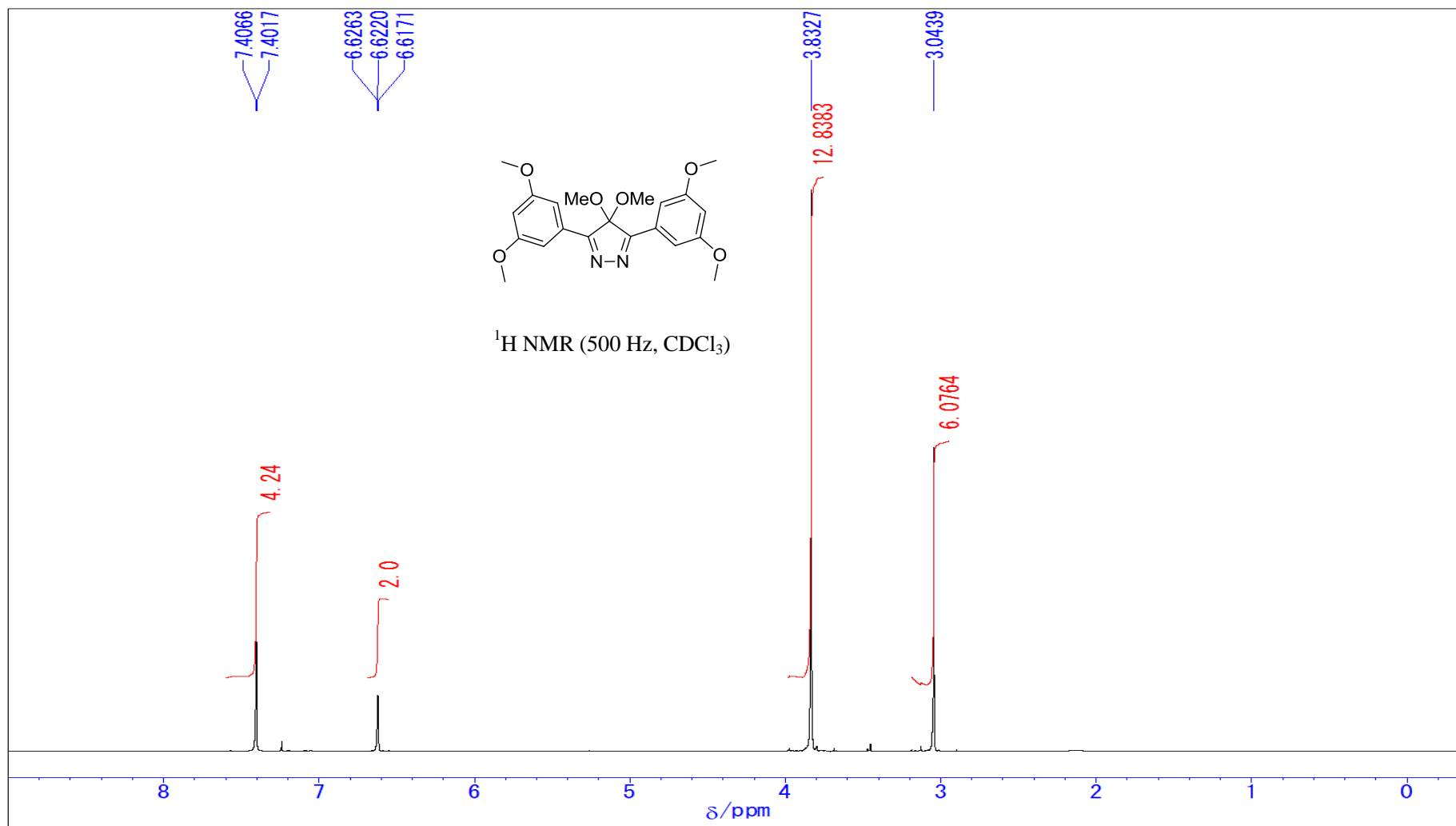




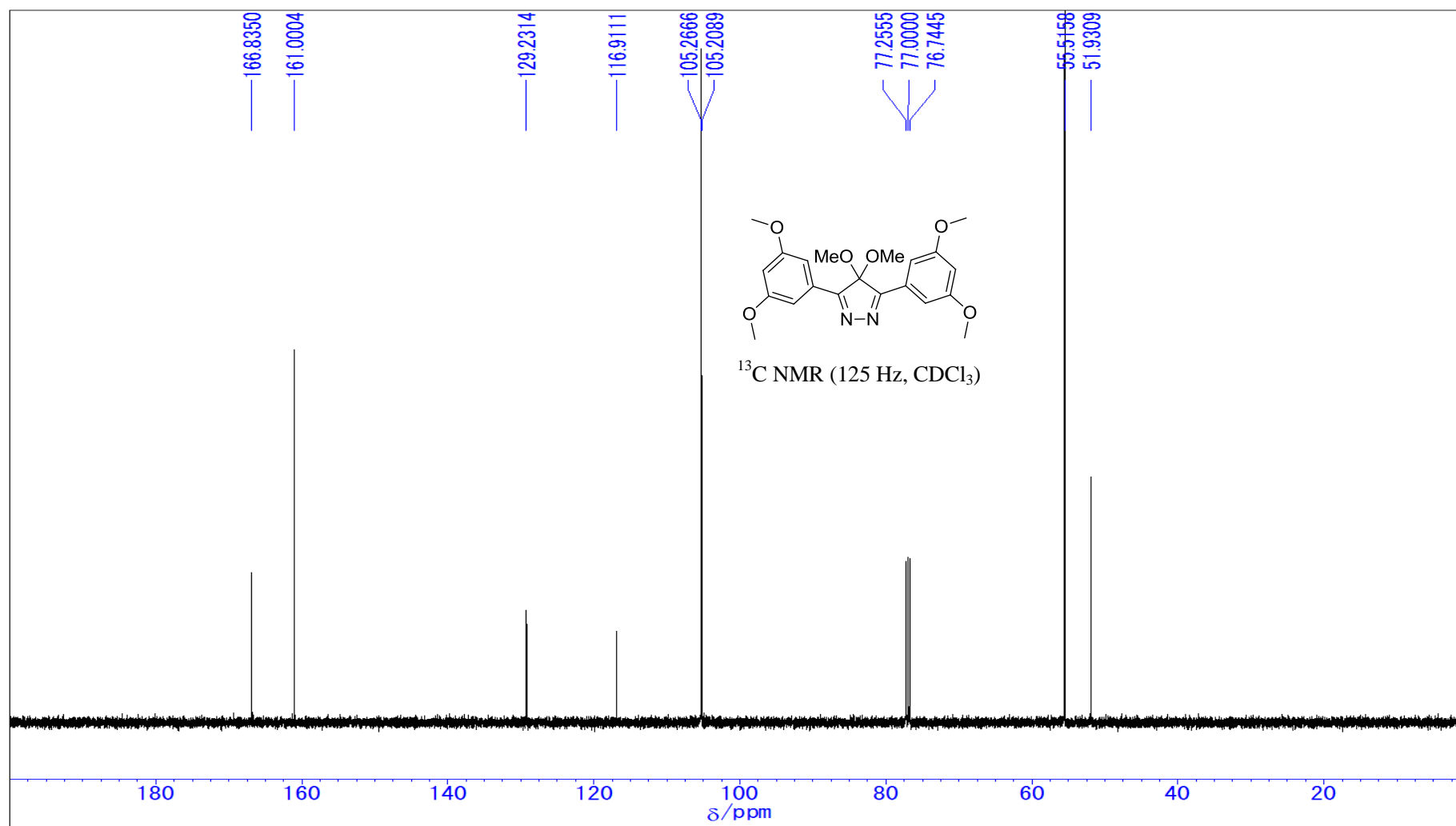
4,4-Bis(3,5-dimethoxybenzyloxy)-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3f)  $^{13}\text{C}$  NMR



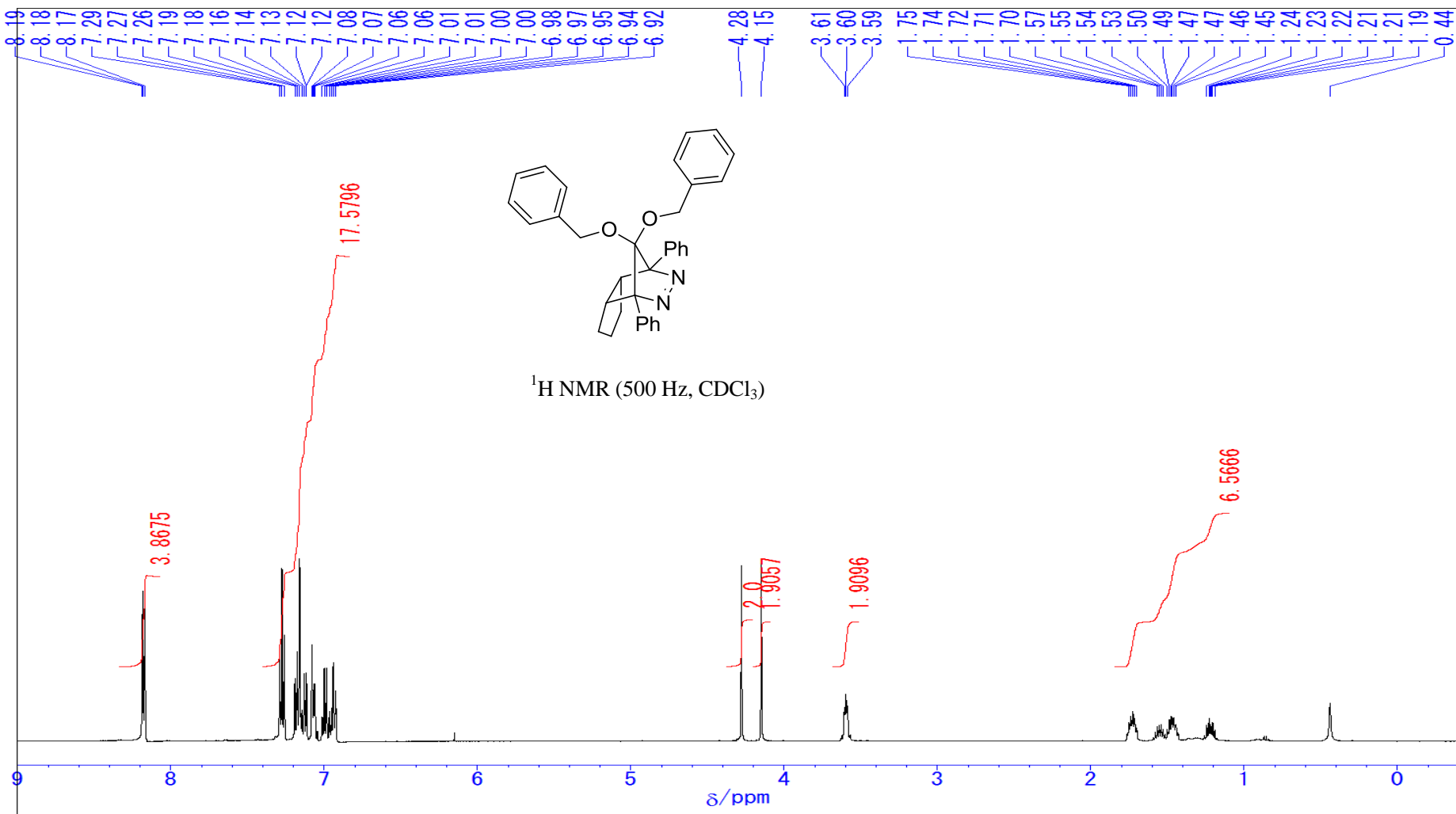
4,4-Dimethoxy-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3g)  $^1\text{H}$  NMR



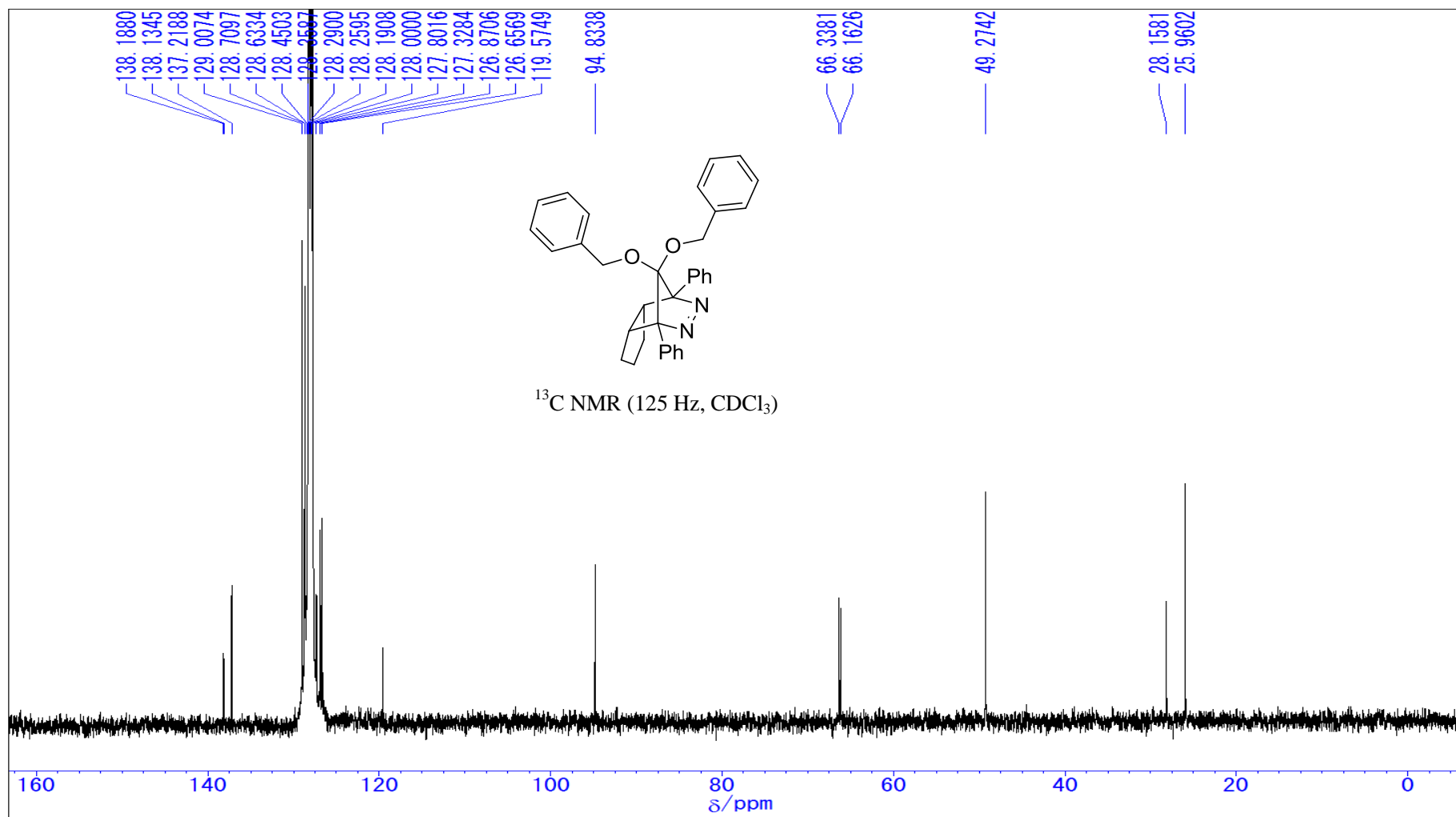
4,4-Dimethoxy-3,5-bis(3,5-dimethoxyphenyl)pyrazole (3g)  $^{13}\text{C}$  NMR



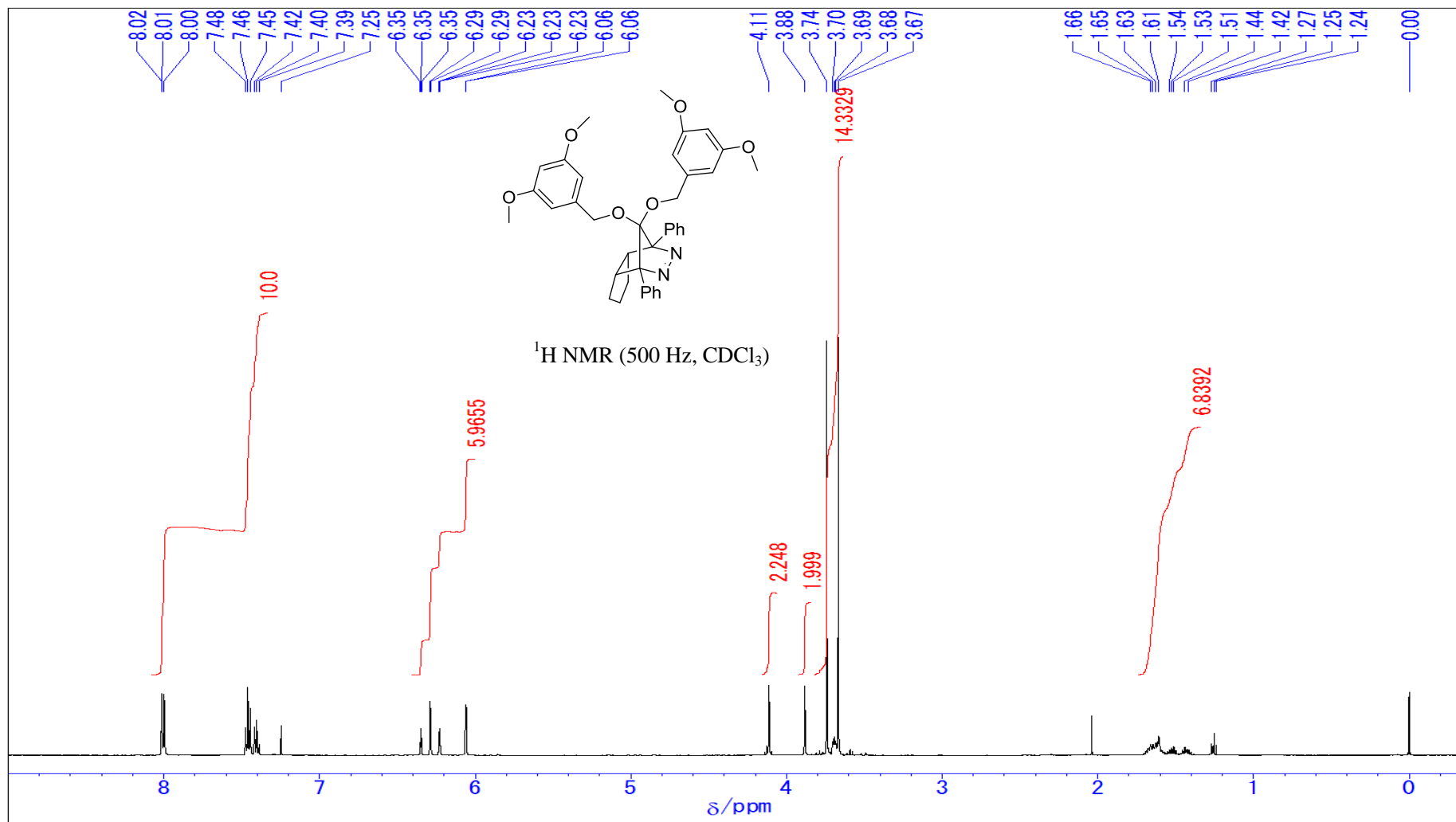
***endo*-2,3-Diazo-10,10-dibenzyloxy-1,4-diphenyltricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZc) <sup>1</sup>H NMR**



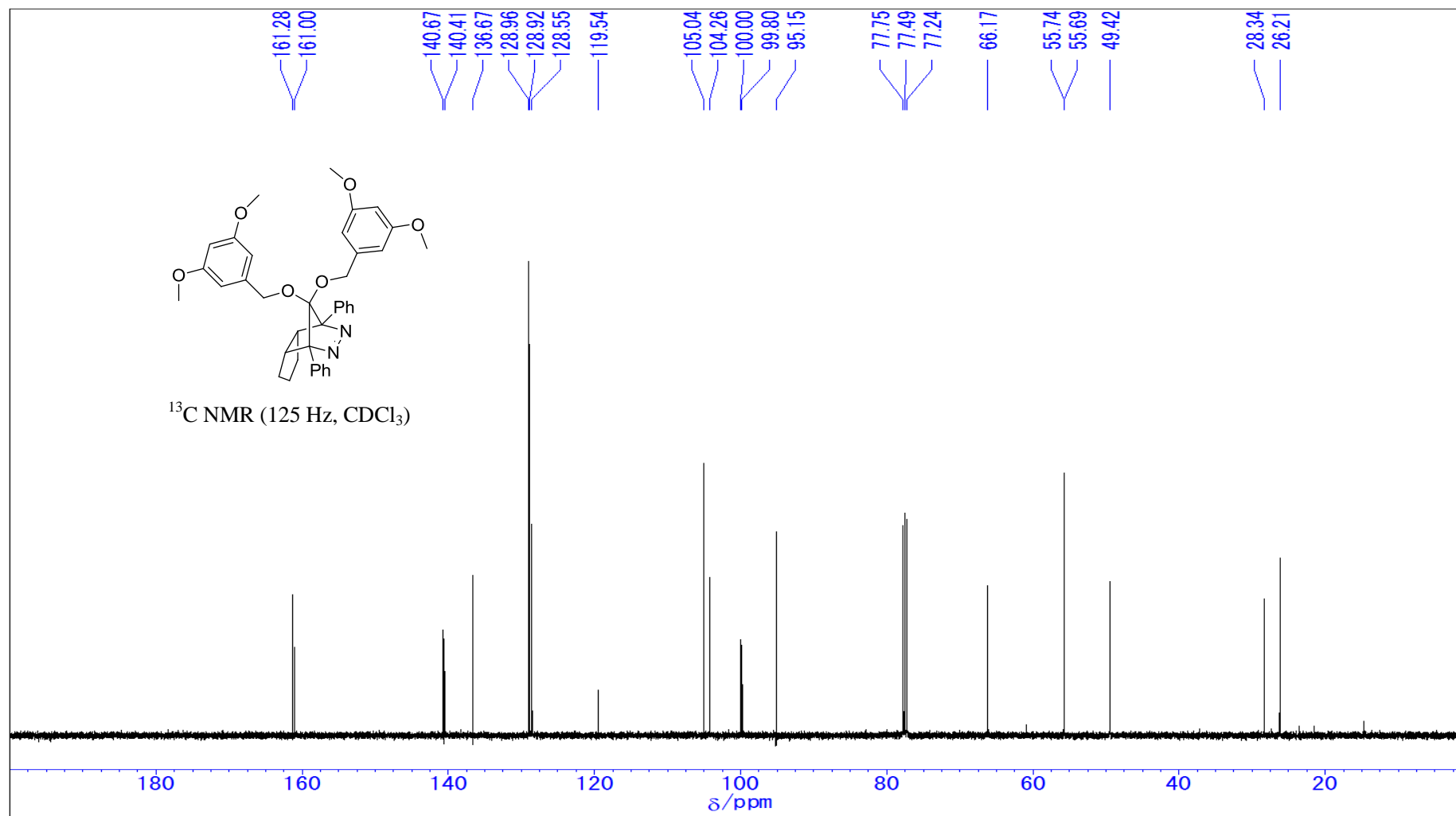
*endo*-2,3-Diazo-10,10-dibenzyloxy-1,4-diphenyltricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZc) <sup>13</sup>C NMR



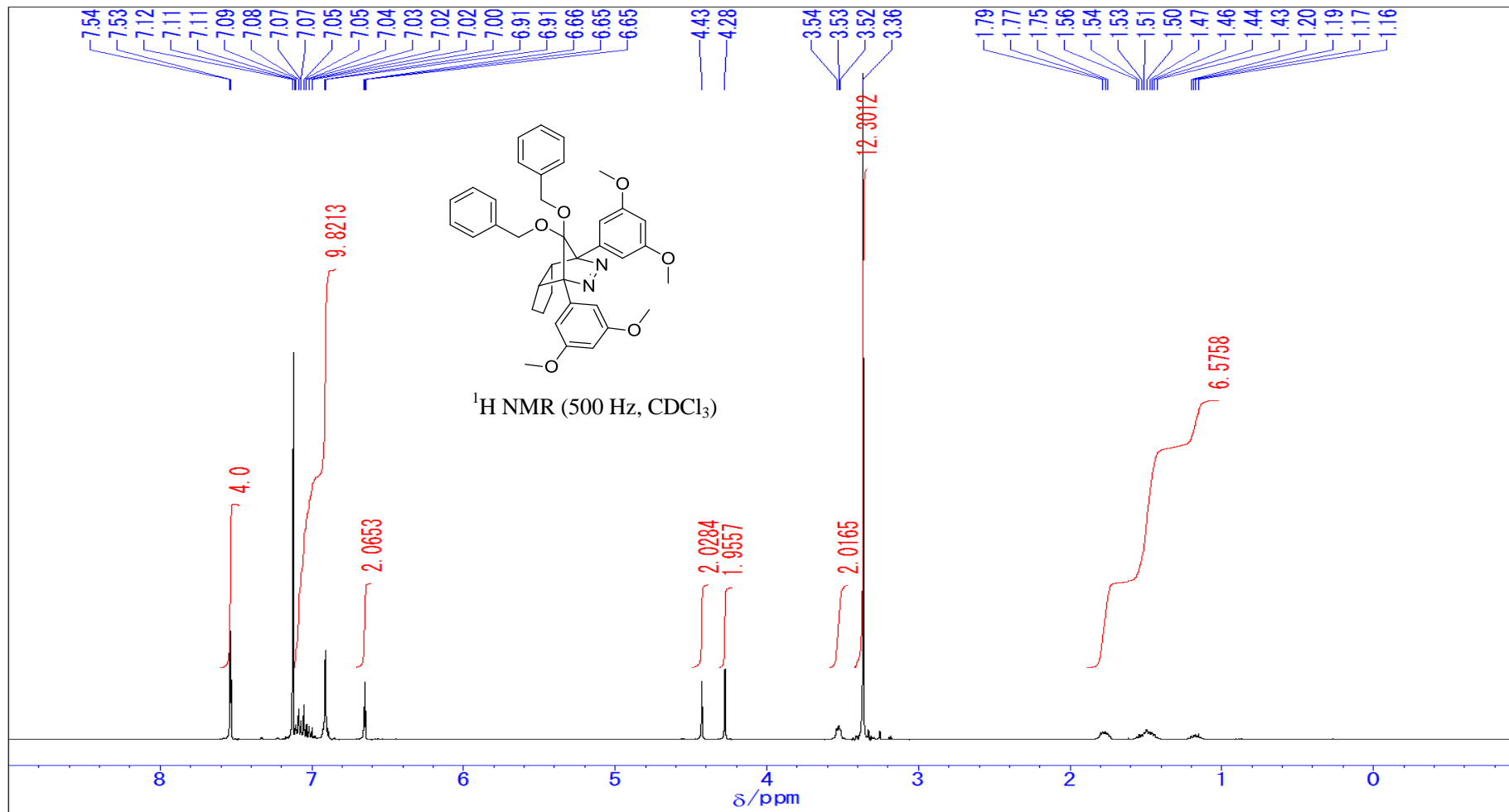
*endo*-2,3-Diazo-10,10-bis(3,5-dimethoxybenzyloxy)-1,4-diphenyltricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZd) <sup>1</sup>H NMR



*endo*-2,3-Diazo-10,10-bis(3,5-dimethoxybenzyloxy)-1,4-diphenyltricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZd) <sup>13</sup>C NMR

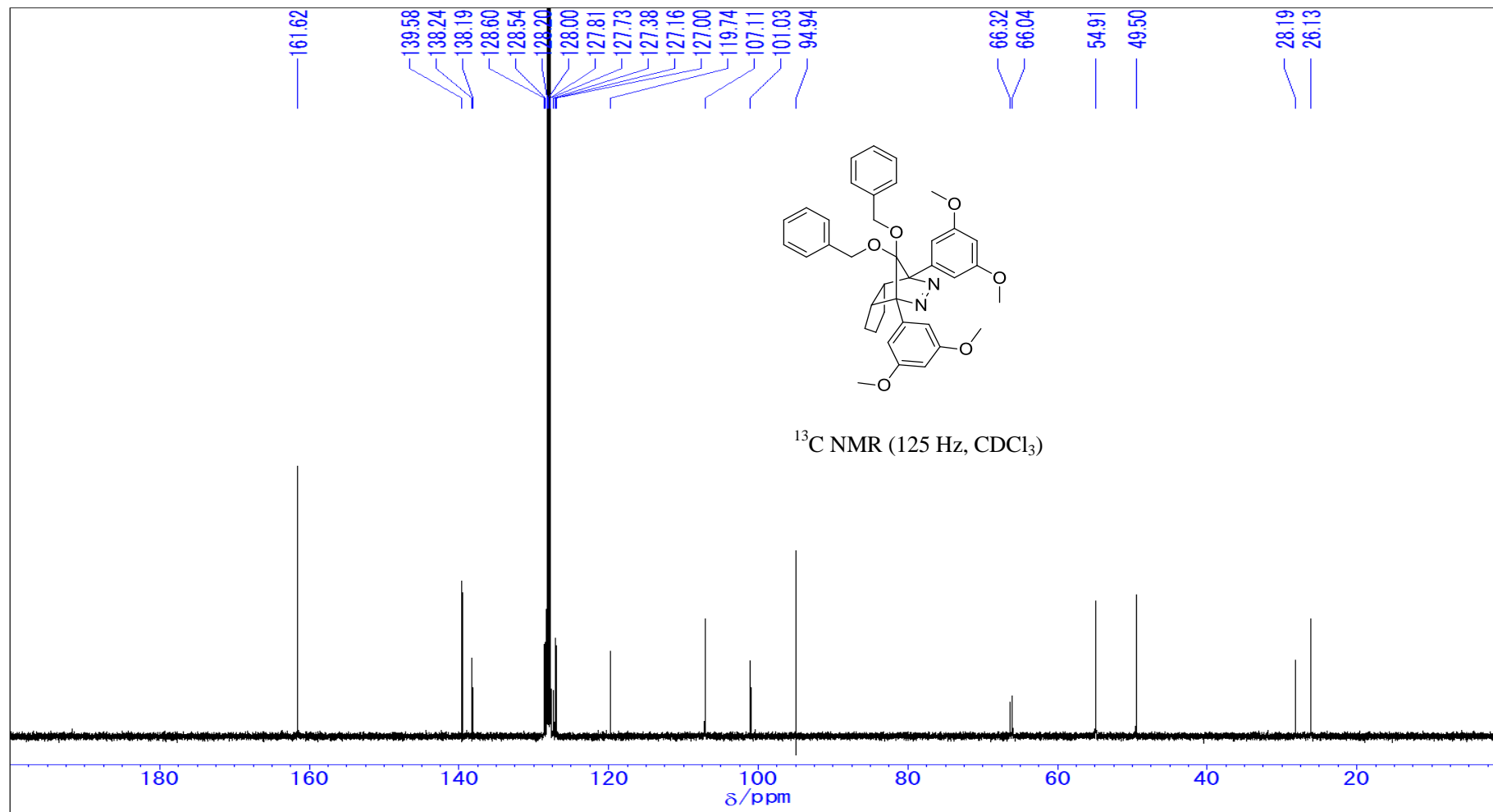


*endo*-2,3-Diazo-1,4-bis(3,5-dimethoxybenzyloxy)-10,10-dibenzyloxytricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZe) <sup>1</sup>H NMR

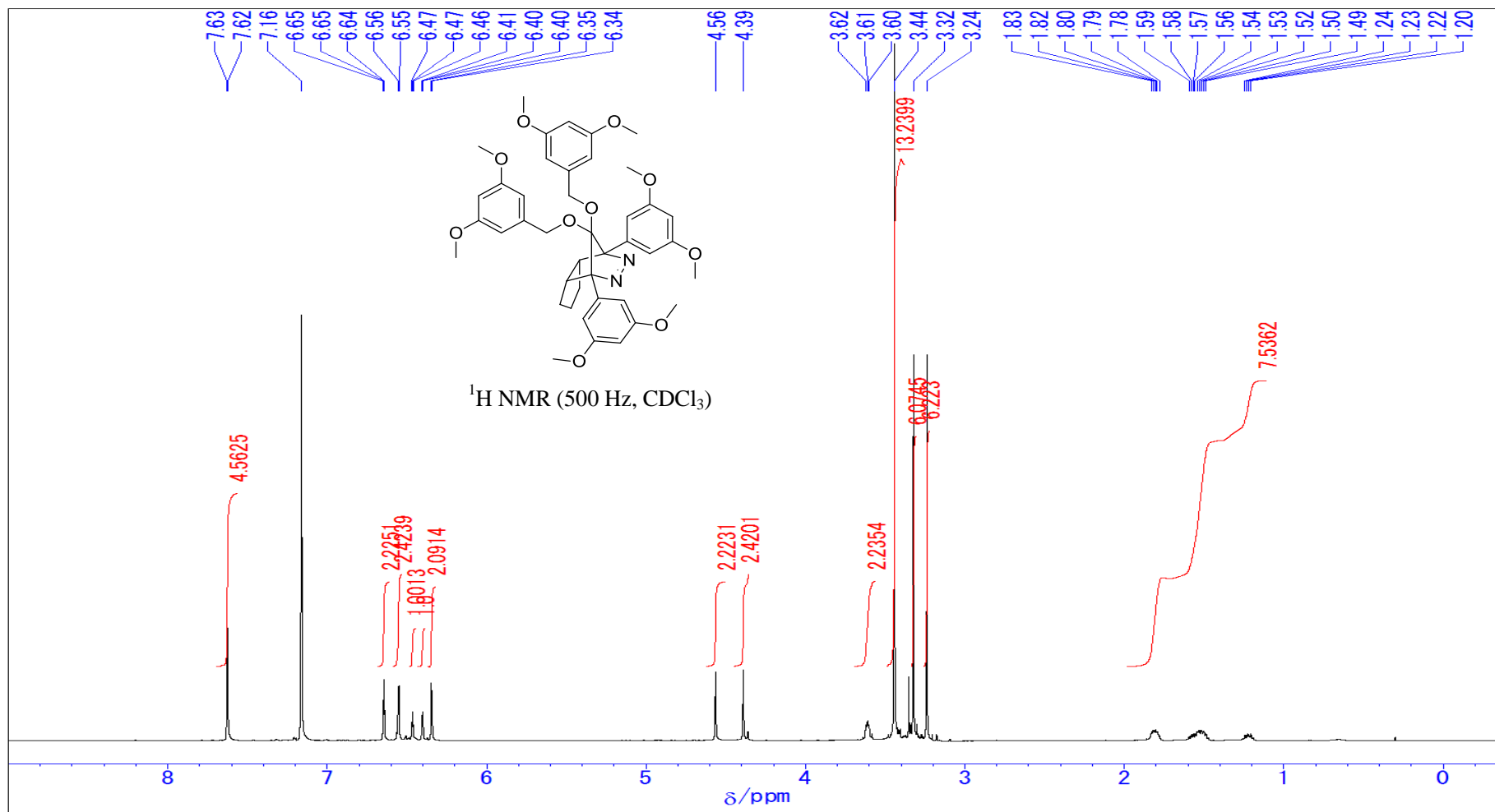




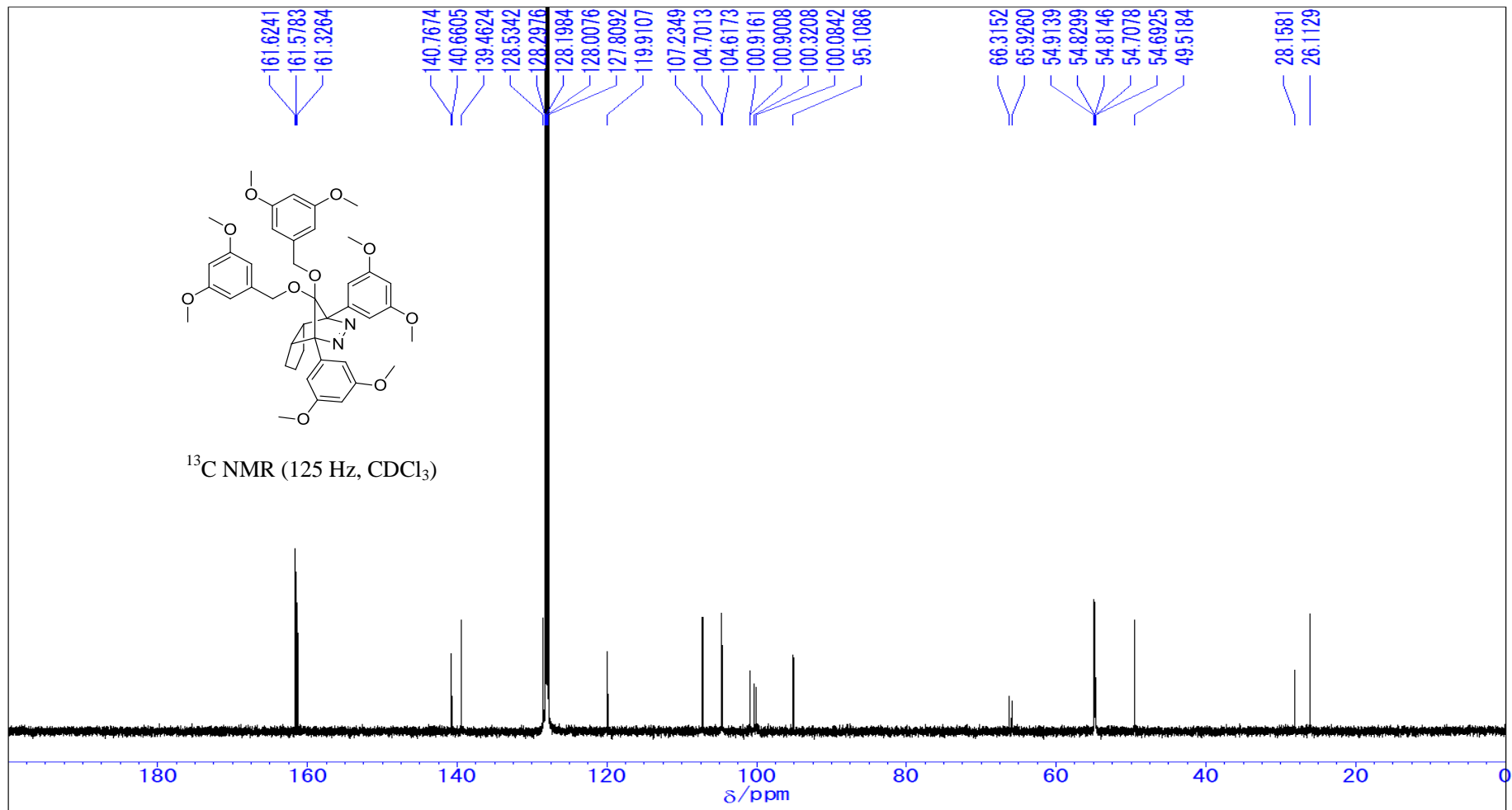
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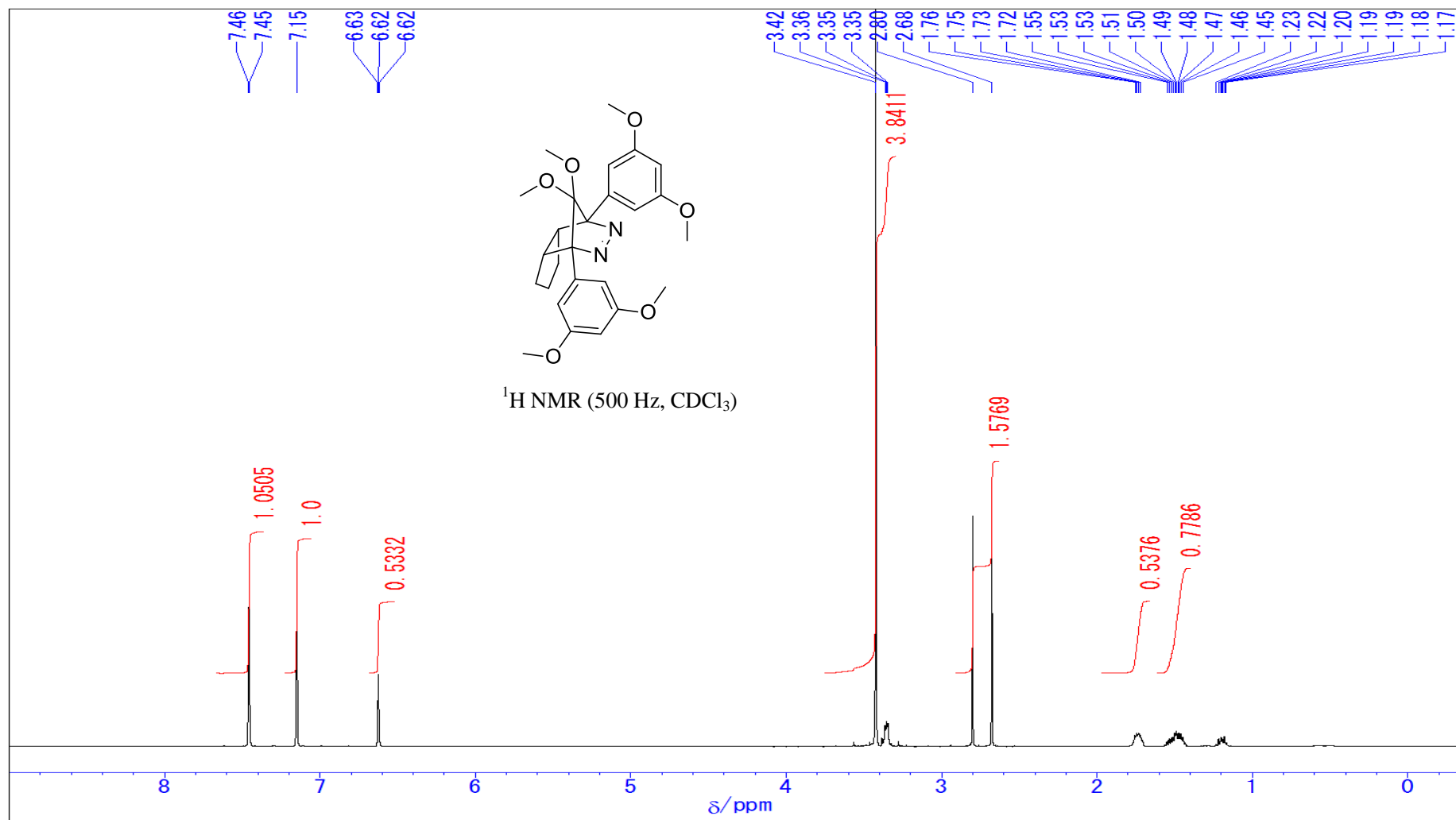
*endo*-2,3-Diazo-1,4-bis(3,5-dimethoxybenzyloxy)-10,10-bis(3,5-dimethoxyphenoxy)tricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZf) <sup>1</sup>H NMR



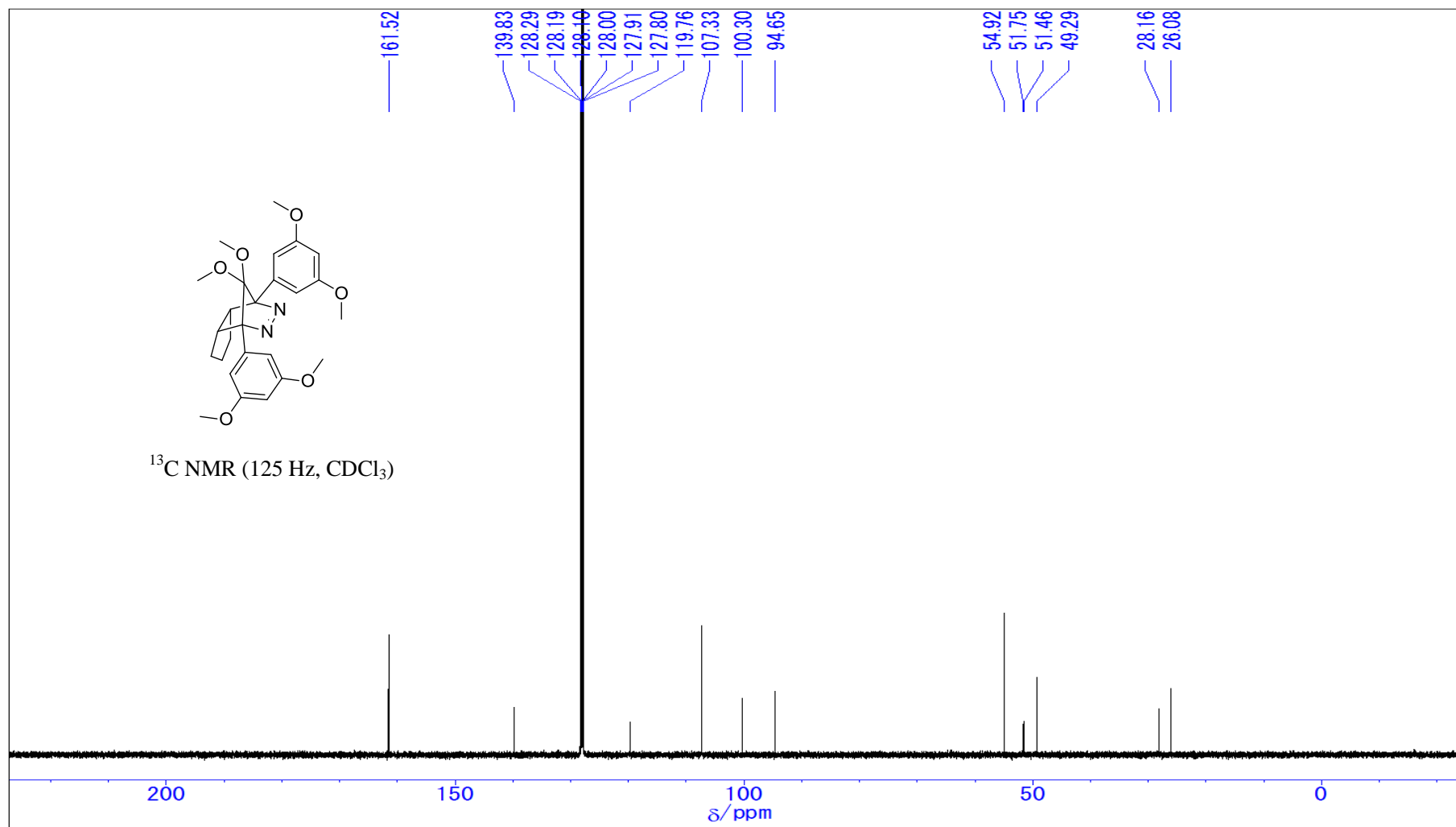
*endo*-2,3-Diazo-1,4-bis(3,5-dimethoxybenzyloxy)-10,10-bis(3,5-dimethoxyphenoxy)tricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZf) <sup>13</sup>C NMR



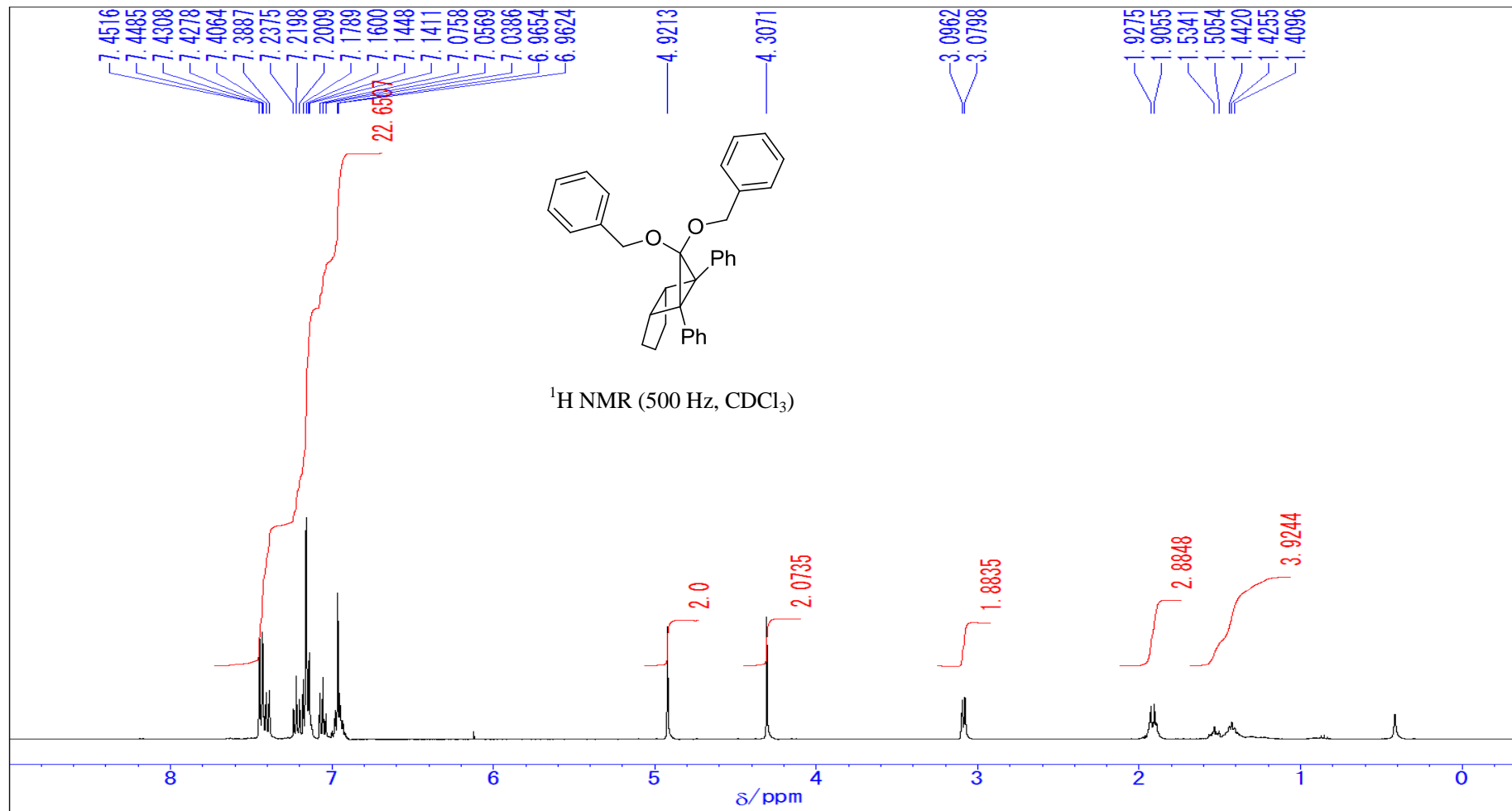
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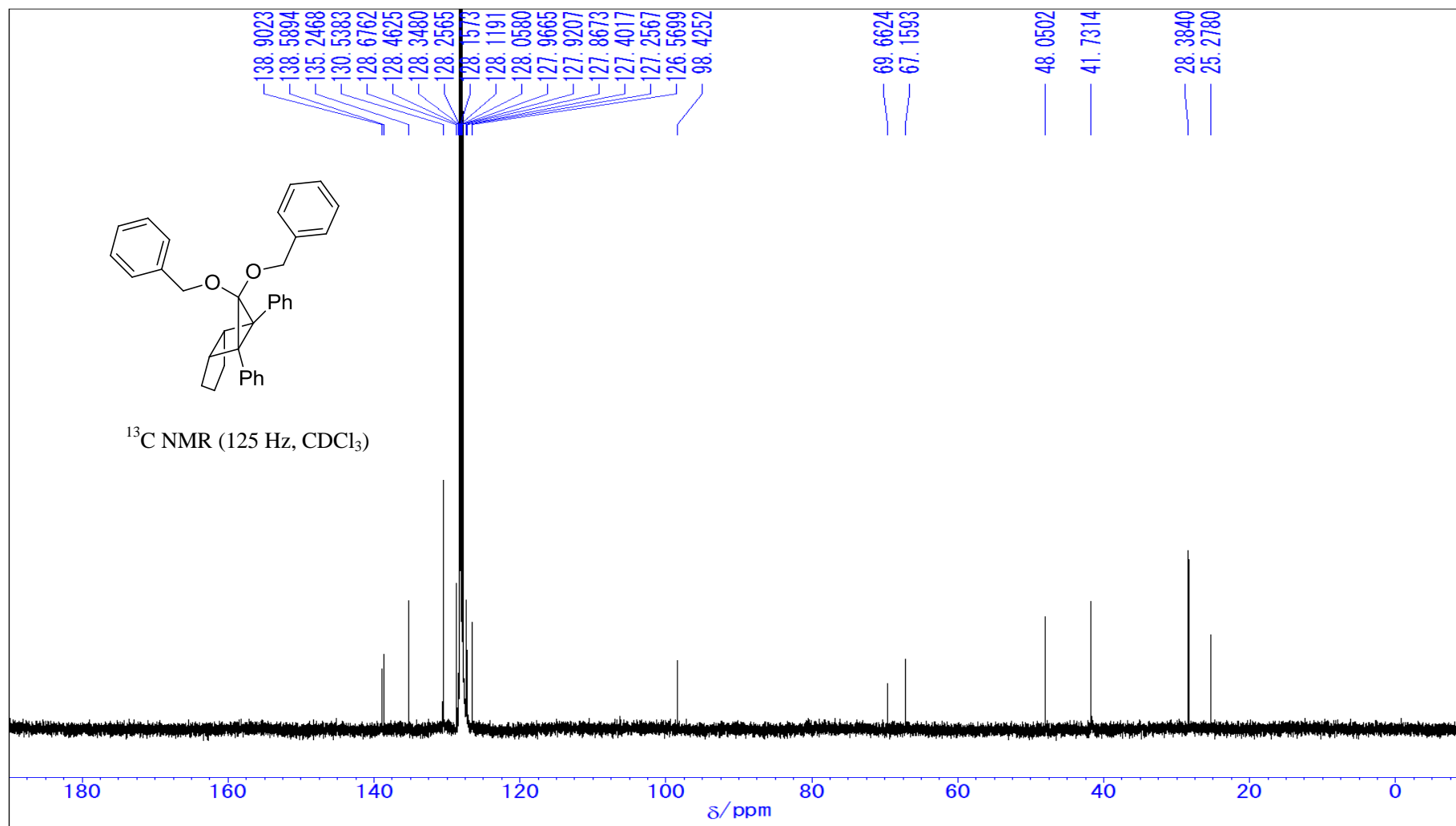
*endo*-2,3-Diazo-1,4-bis(3,5-dimethoxybenzyloxy)-10,10-dimethoxytricyclo[5.2.1.0<sup>5,9</sup>]dec-2-ene (AZg) <sup>13</sup>C NMR



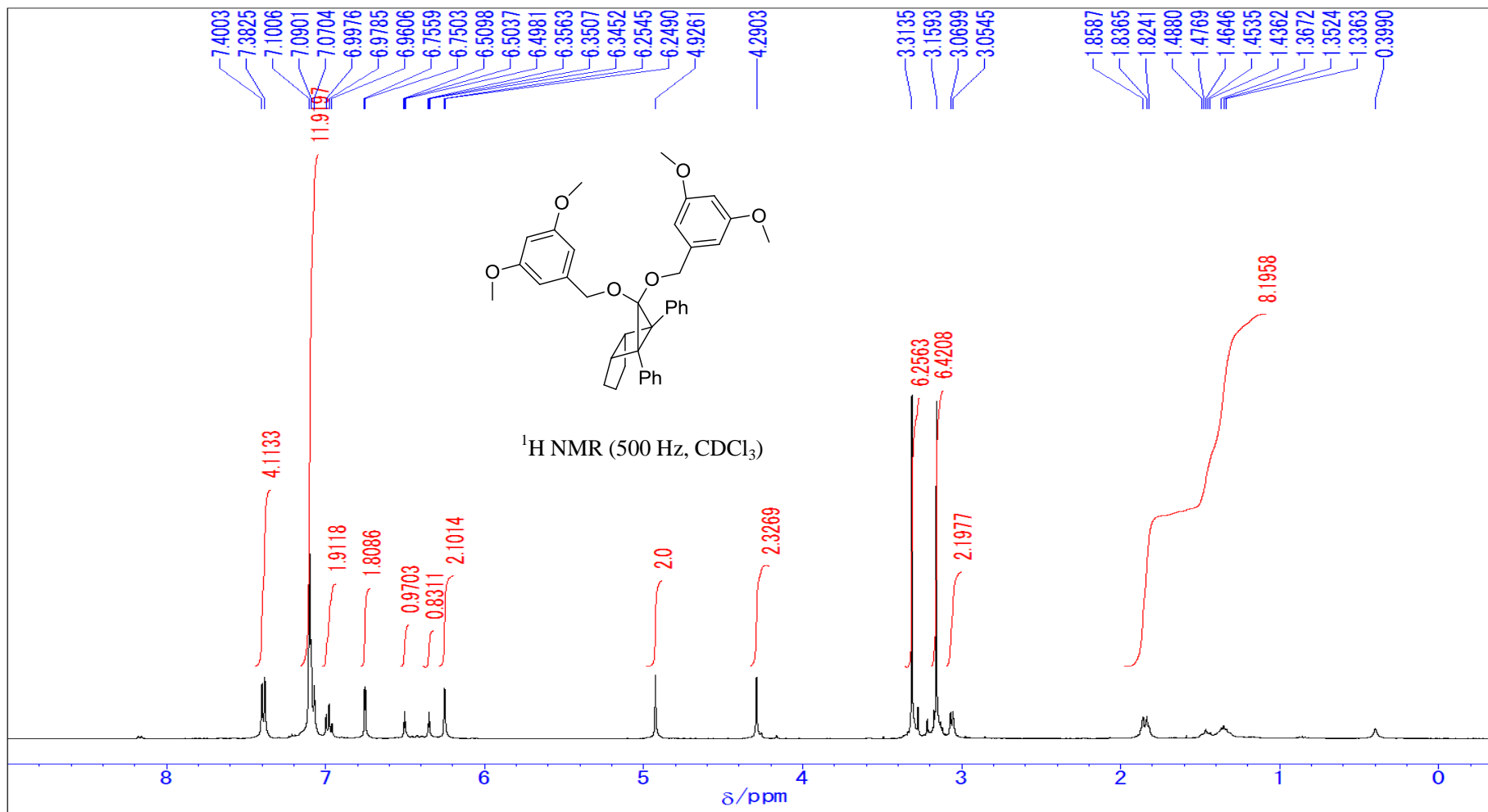
3,3-Dibenzyloxy-2,4-diphenyltricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPC) <sup>1</sup>H NMR



3,3-Dibenzyloxy-2,4-diphenyltricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPc) <sup>13</sup>C NMR

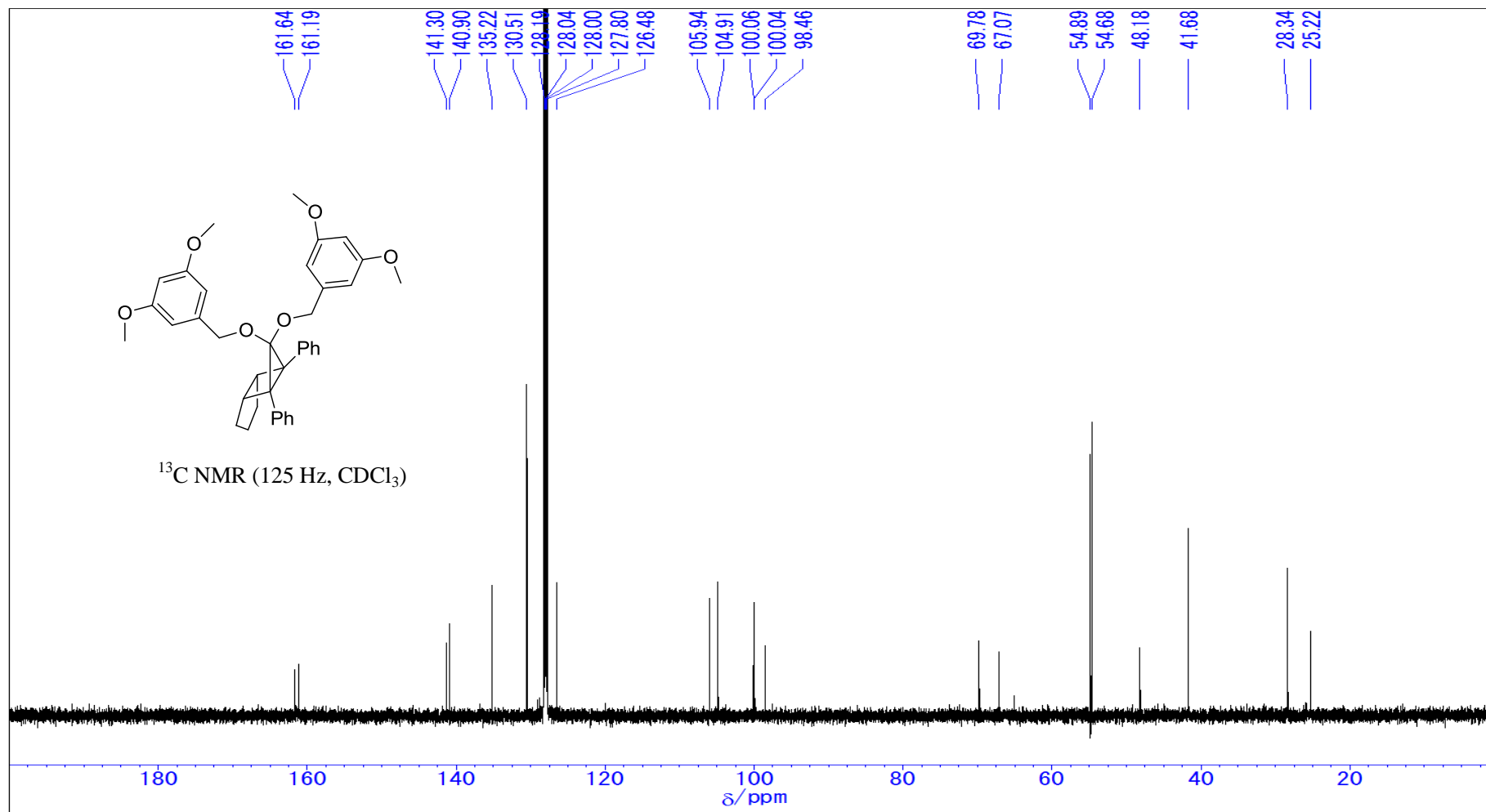


3,3-Bis(3,5-dimethoxybenzyloxy)-2,4-diphenyltricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPd) <sup>1</sup>H NMR

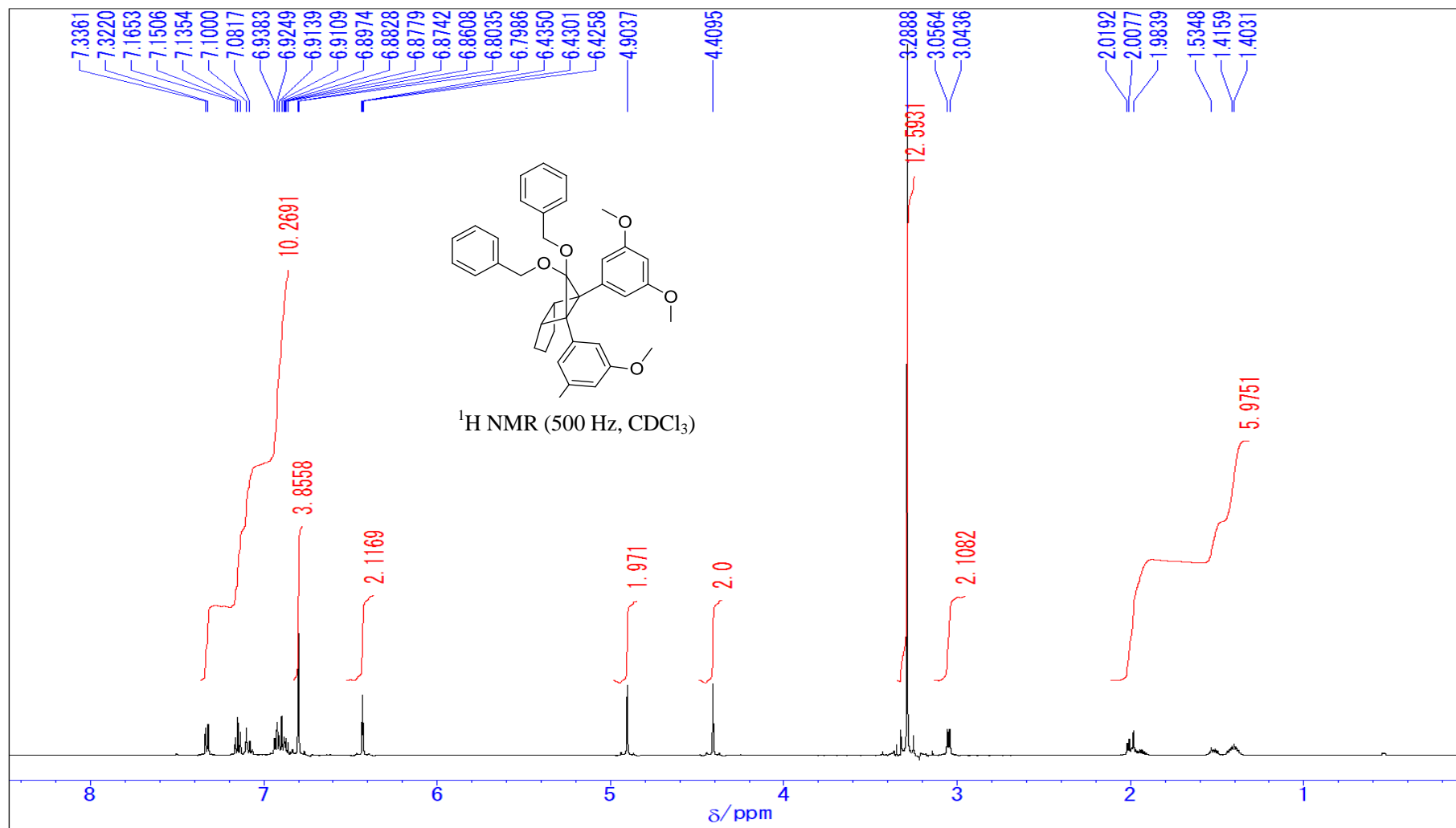




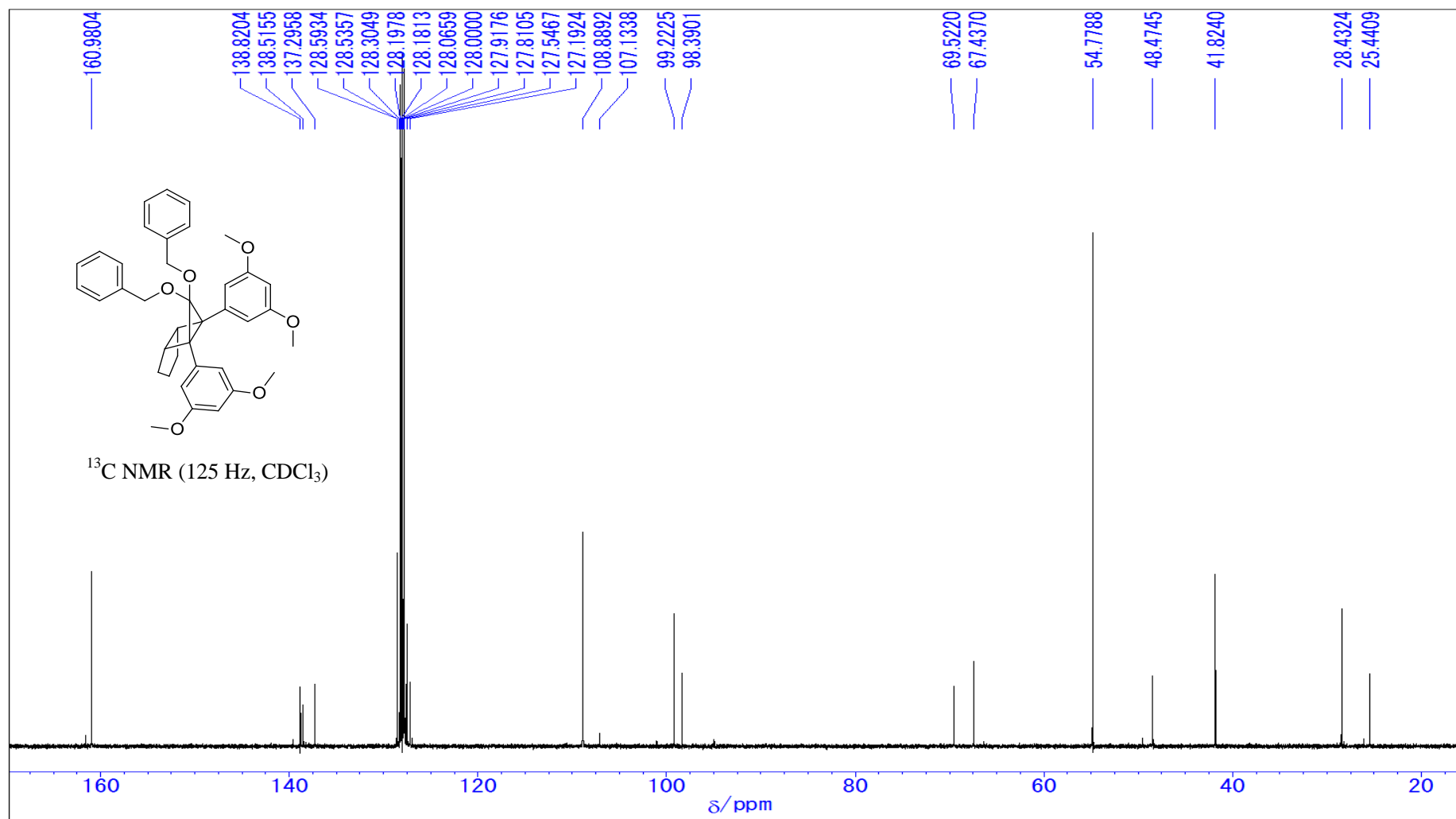
**3,3-Bis(3,5-dimethoxybenzyloxy)-2,4-diphenyltricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPd) <sup>13</sup>C NMR**



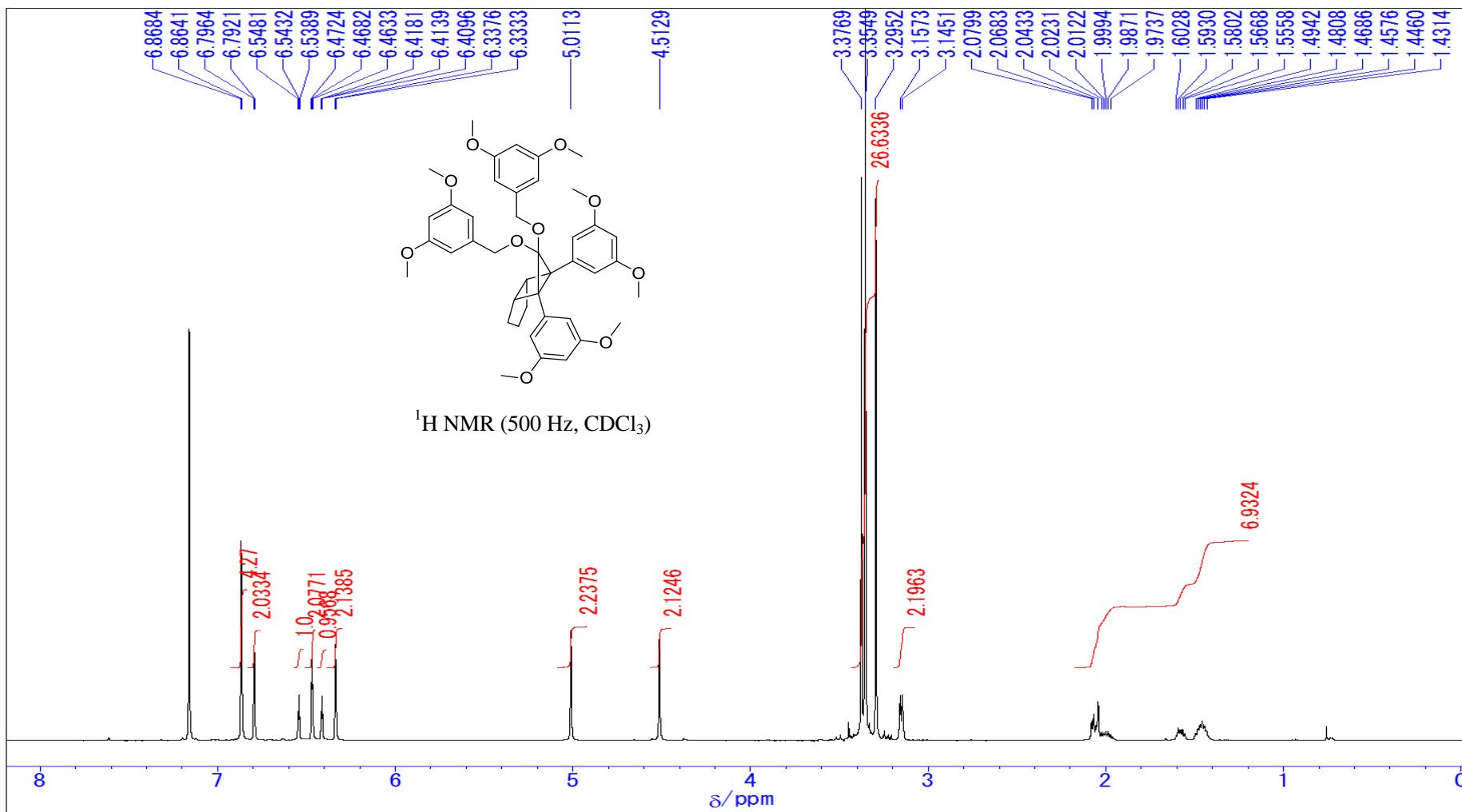
3,3-Dibenzyloxy-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPe) <sup>1</sup>H NMR



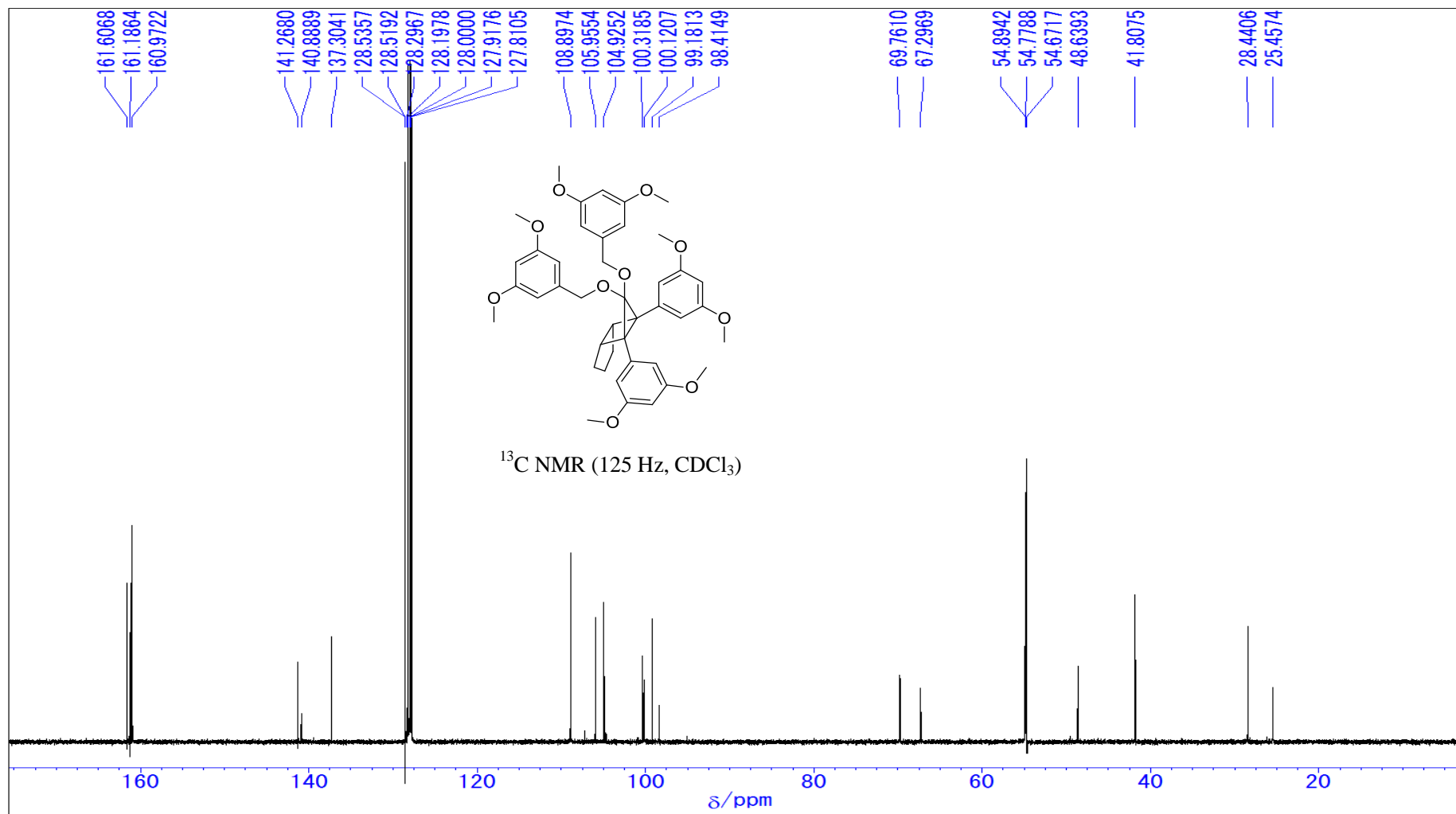
3,3-Dibenzyloxy-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPe) <sup>13</sup>C NMR



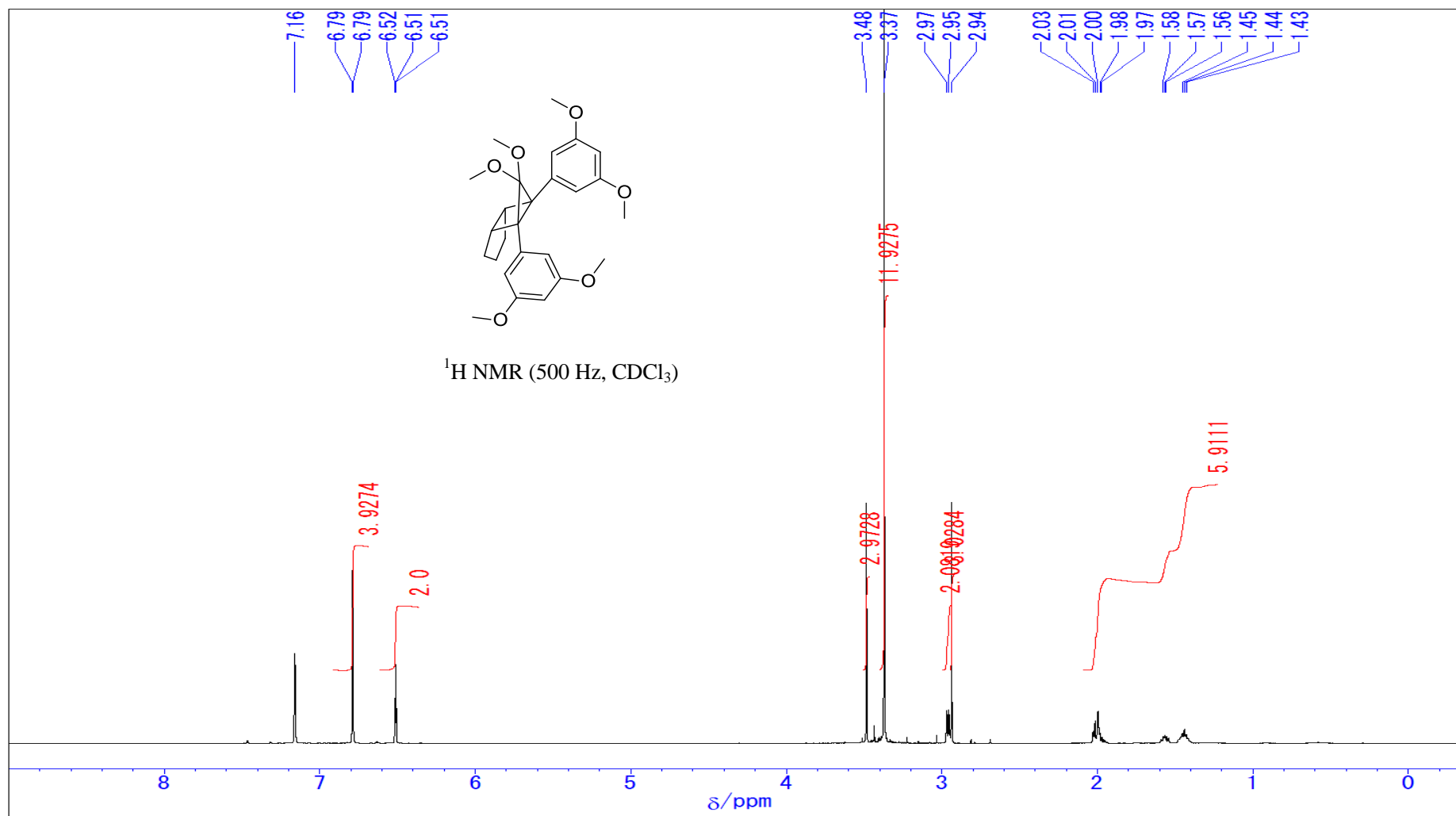
**3,3-Bis(3,5-dimethoxybenzyloxy)-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPf) <sup>1</sup>H NMR**



**3,3-Bis(3,5-dimethoxybenzyloxy)-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPf) <sup>13</sup>C NMR**



3,3-Dimethoxy-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPg) <sup>1</sup>H NMR



3,3-Dimethoxy-2,4-bis(3,5-dimethoxyphenyl)tricyclo[3.3.0.<sup>1,5</sup>0<sup>2,4</sup>]octane (CPg) <sup>13</sup>C NMR

