

## Supplementary Material

### Iron nitrate/TEMPO-catalyzed oxidative Passerini reaction of alcohols in air

Shivalinga Kolle,<sup>a</sup> Shashikant U. Dighe,<sup>a</sup> and Sanjay Batra<sup>\*a,b</sup>

<sup>a</sup> Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute,  
BS-10/1, Sector 10, Jankipuram Extension, Sitapur Road, Lucknow 226031, India

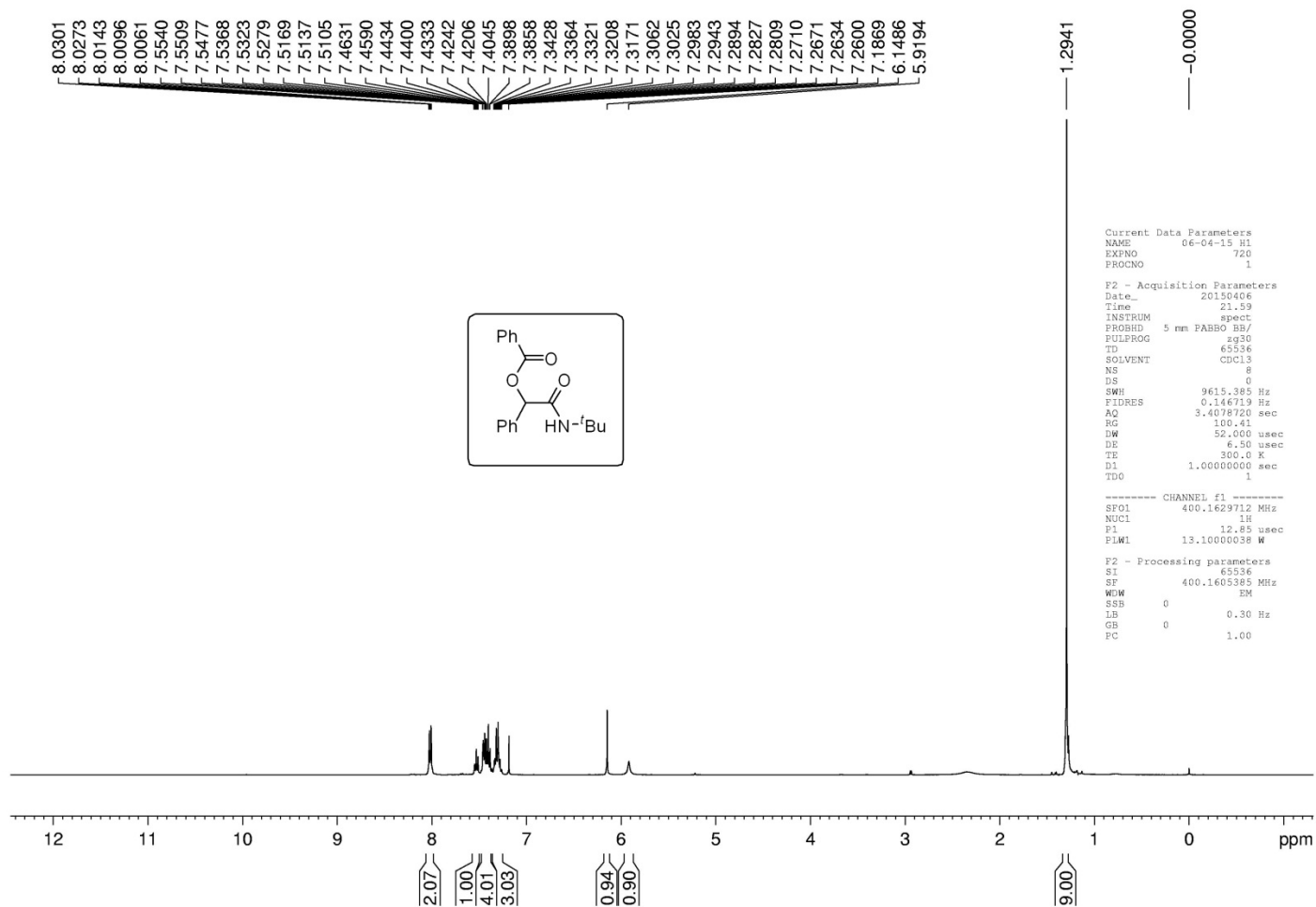
<sup>b</sup> Academy of Scientific and Innovative Research, New Delhi 110025, India

E-mail: [batra\\_san@yahoo.co.uk](mailto:batra_san@yahoo.co.uk), [s\\_batra@cdri.res.in](mailto:s_batra@cdri.res.in)

Dedicated to Dr. Jhillu Singh Yadav on the occasion of his 65<sup>th</sup> anniversary

#### Contents

1. Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of Compounds S-2

Copies  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR Spectra of Compounds:Figure S1.  $^1\text{H}$ -NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl benzoate (4aAa).

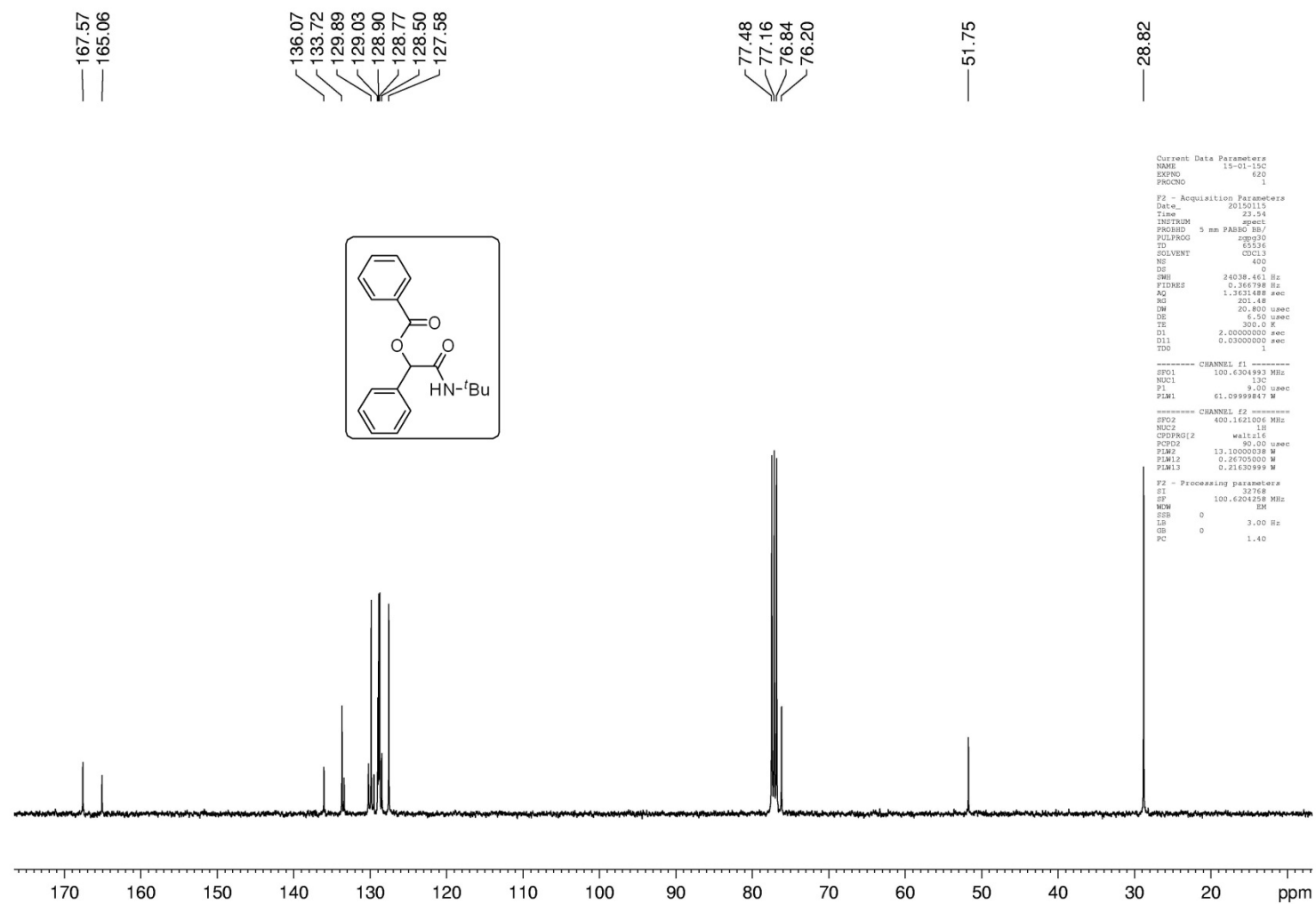
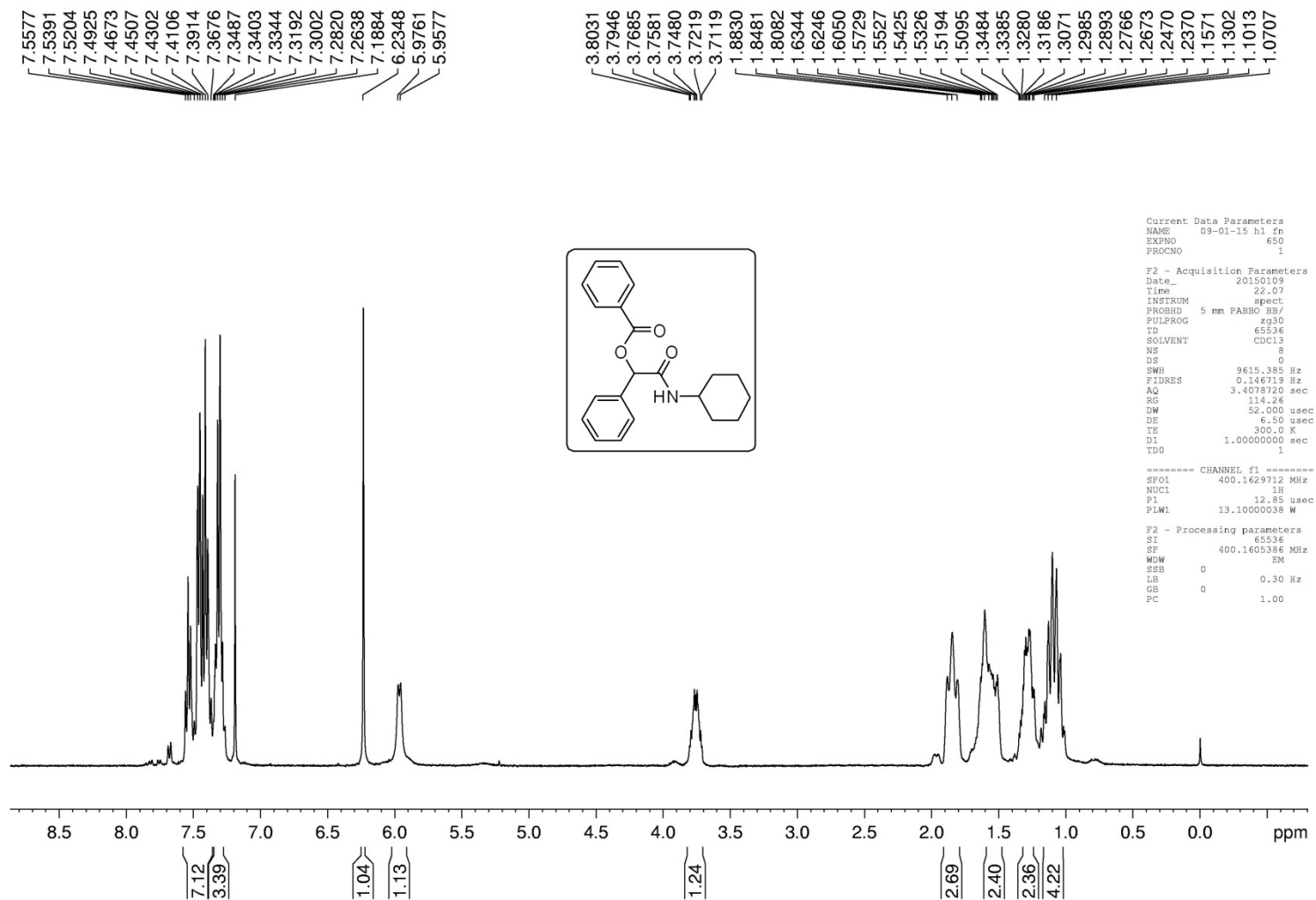
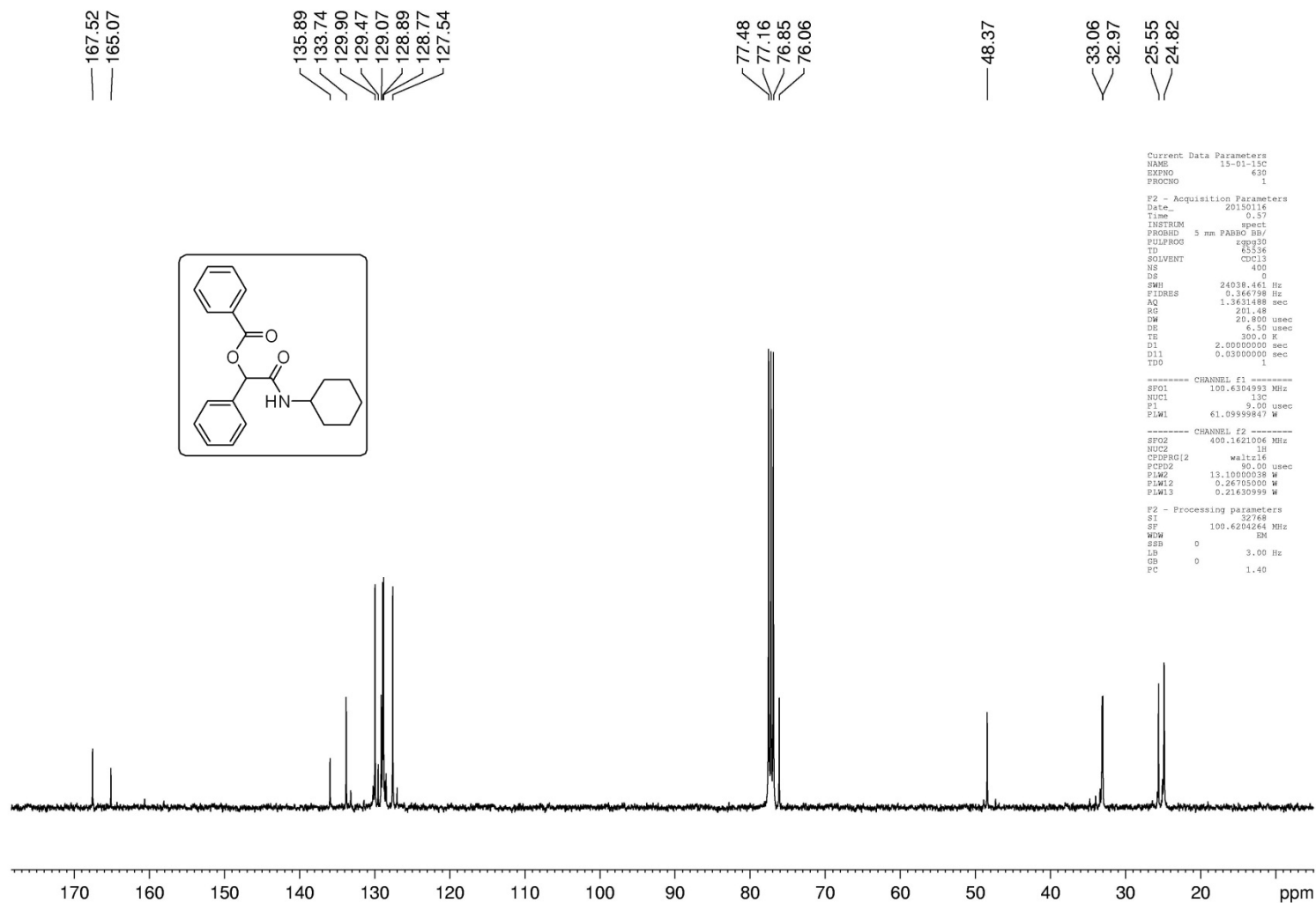


Figure S2. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl benzoate (4aAa).



**Figure S3.** <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl benzoate (**4aAb**).



**Figure S4.** <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl benzoate (**4aAb**).

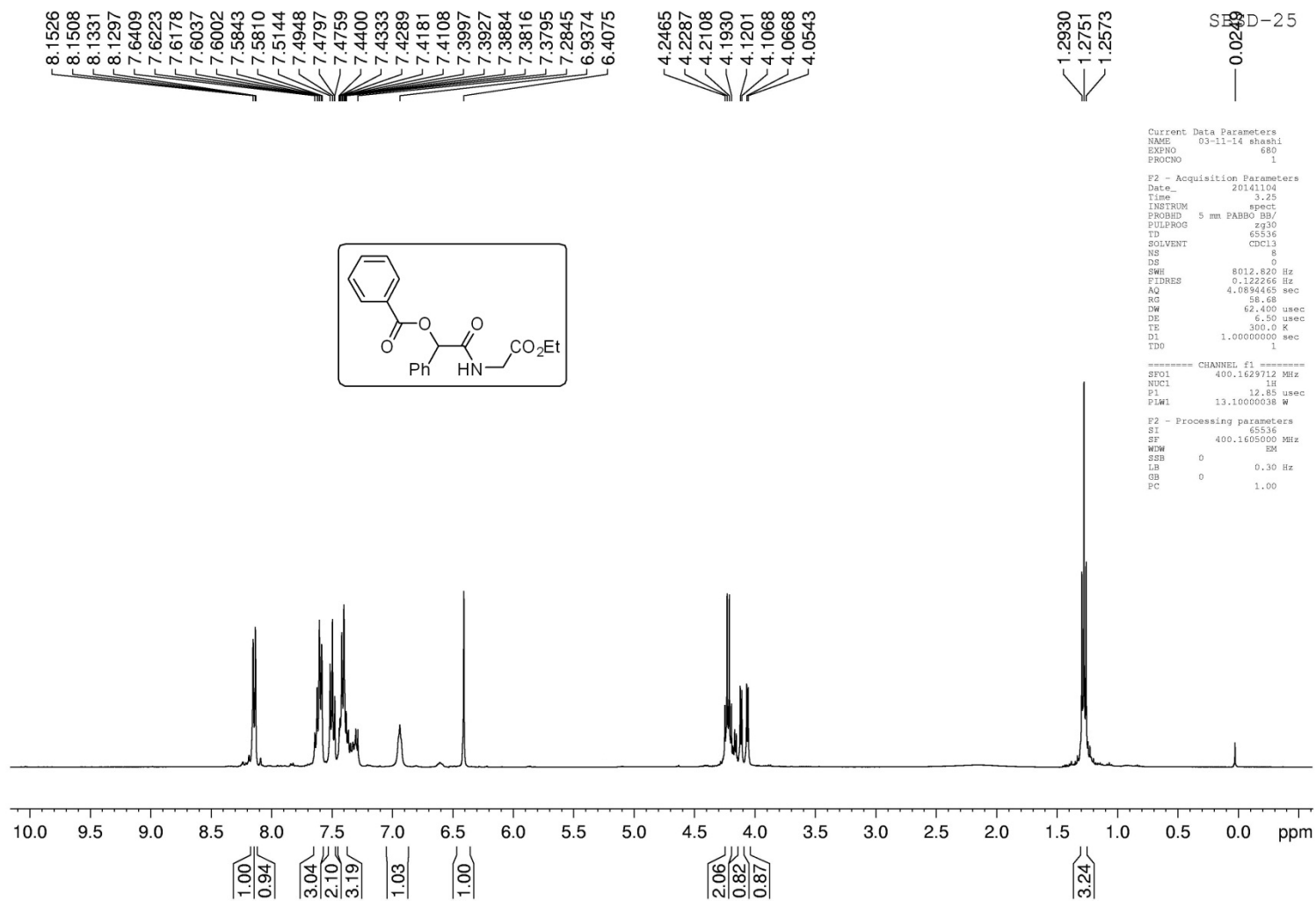
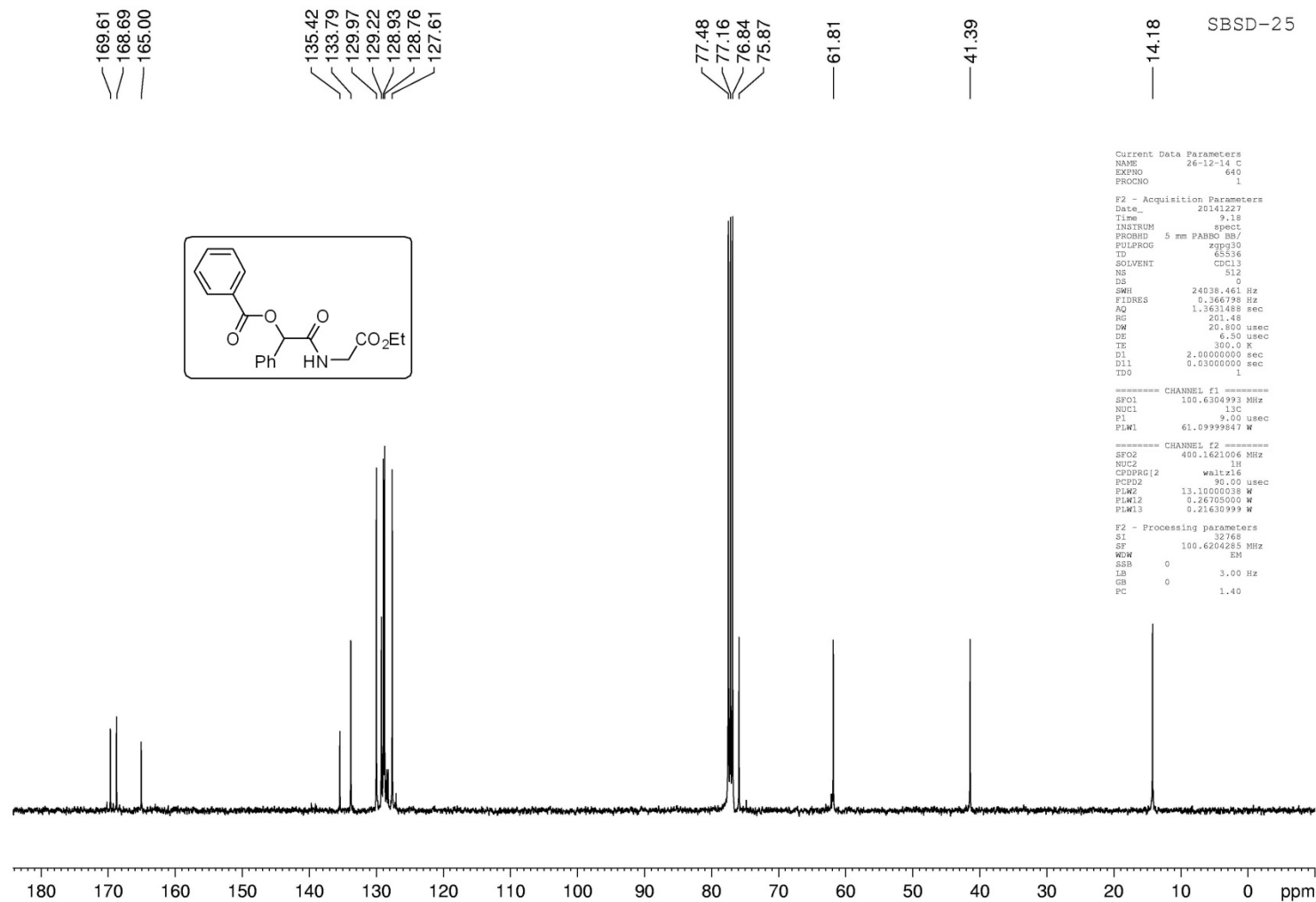
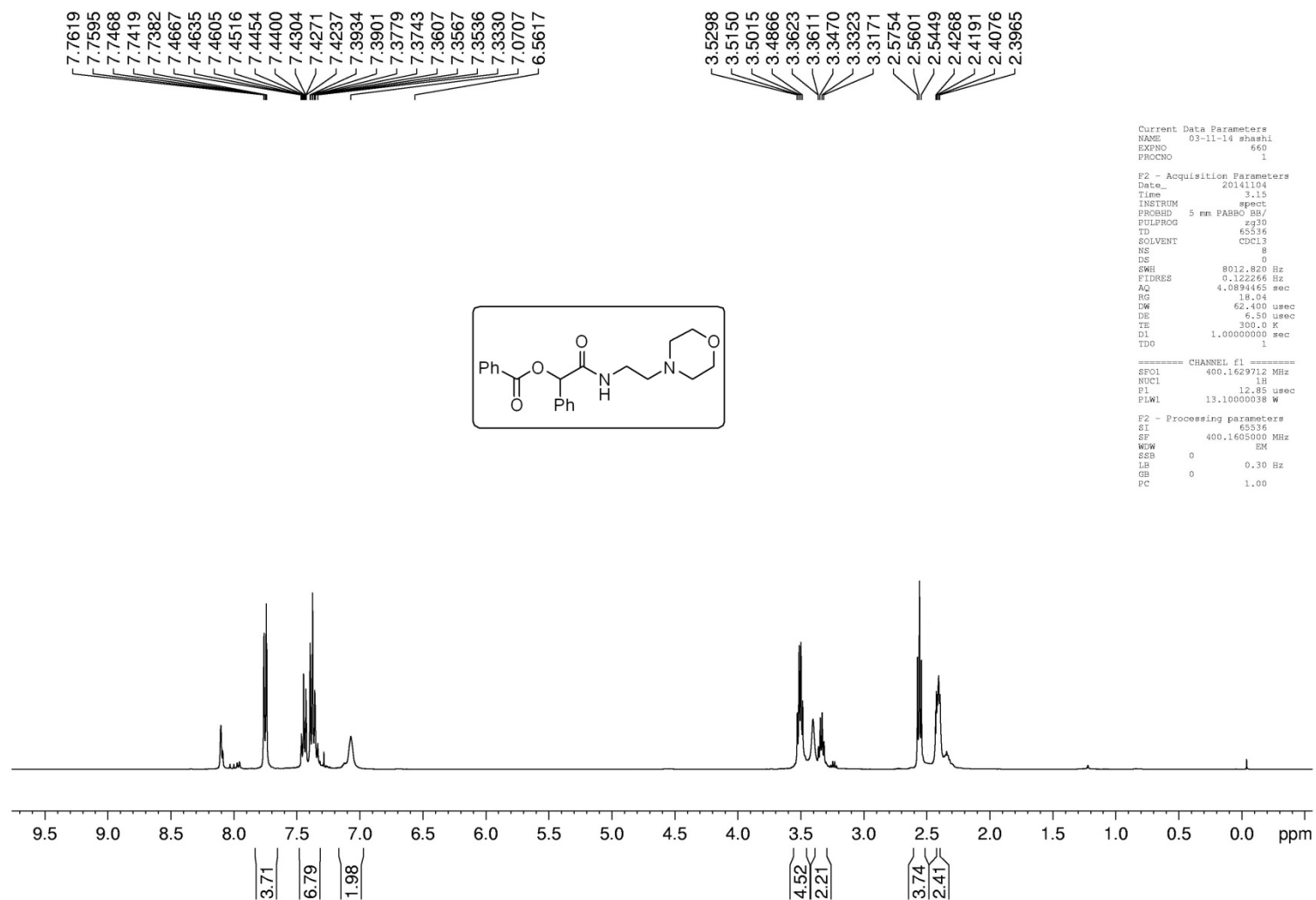


Figure S5. <sup>1</sup>H-NMR spectrum of 2-((2-ethoxy-2-oxoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAc**).



**Figure S6.**  $^{13}\text{C}$ -NMR spectrum of 2-((2-ethoxy-2-oxoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAc**).



**Figure S7.** <sup>1</sup>H-NMR spectrum of 2-((2-morpholinoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAd**).



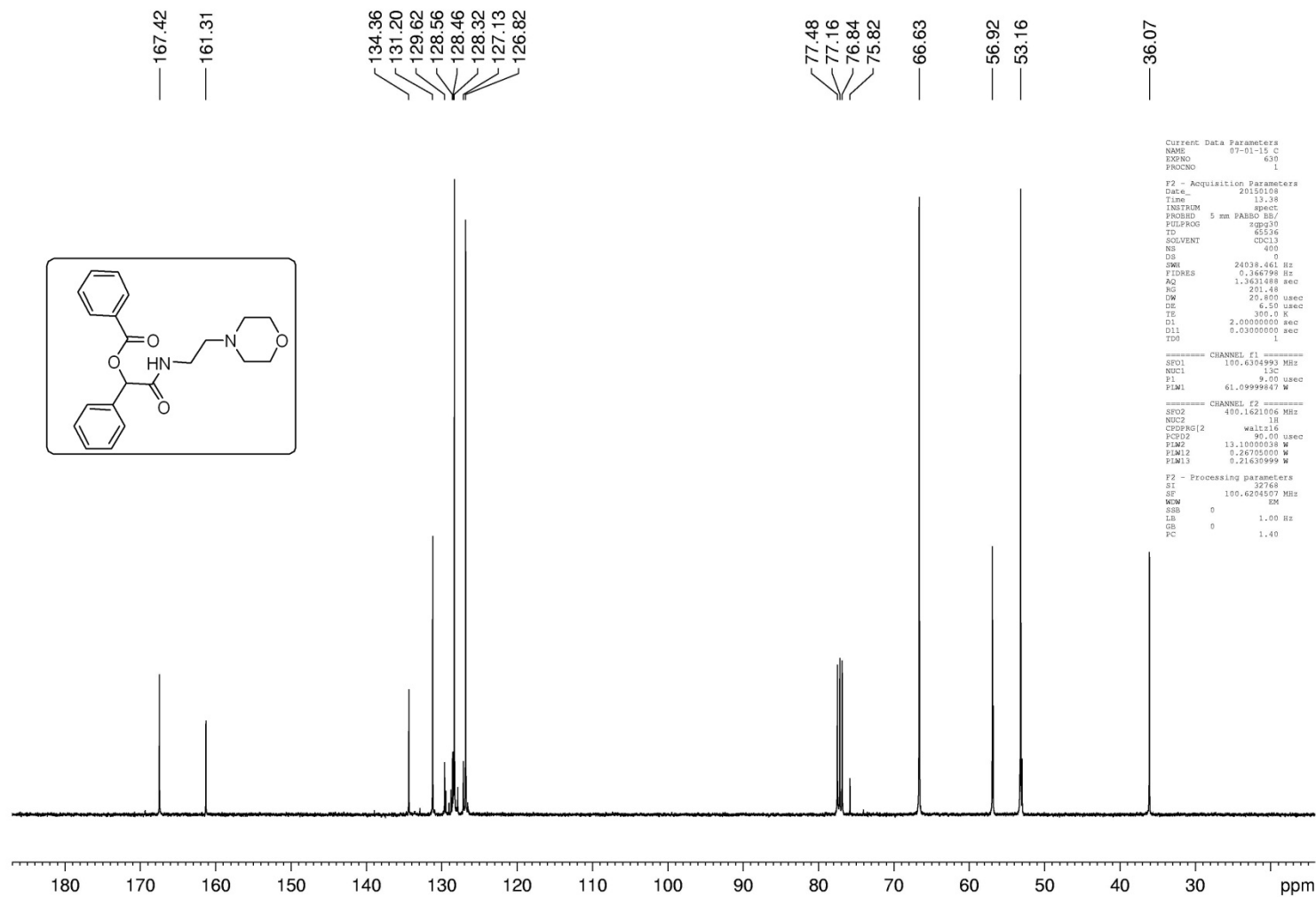


Figure S8. <sup>13</sup>C-NMR spectrum of 2-((2-morpholinoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAd**).

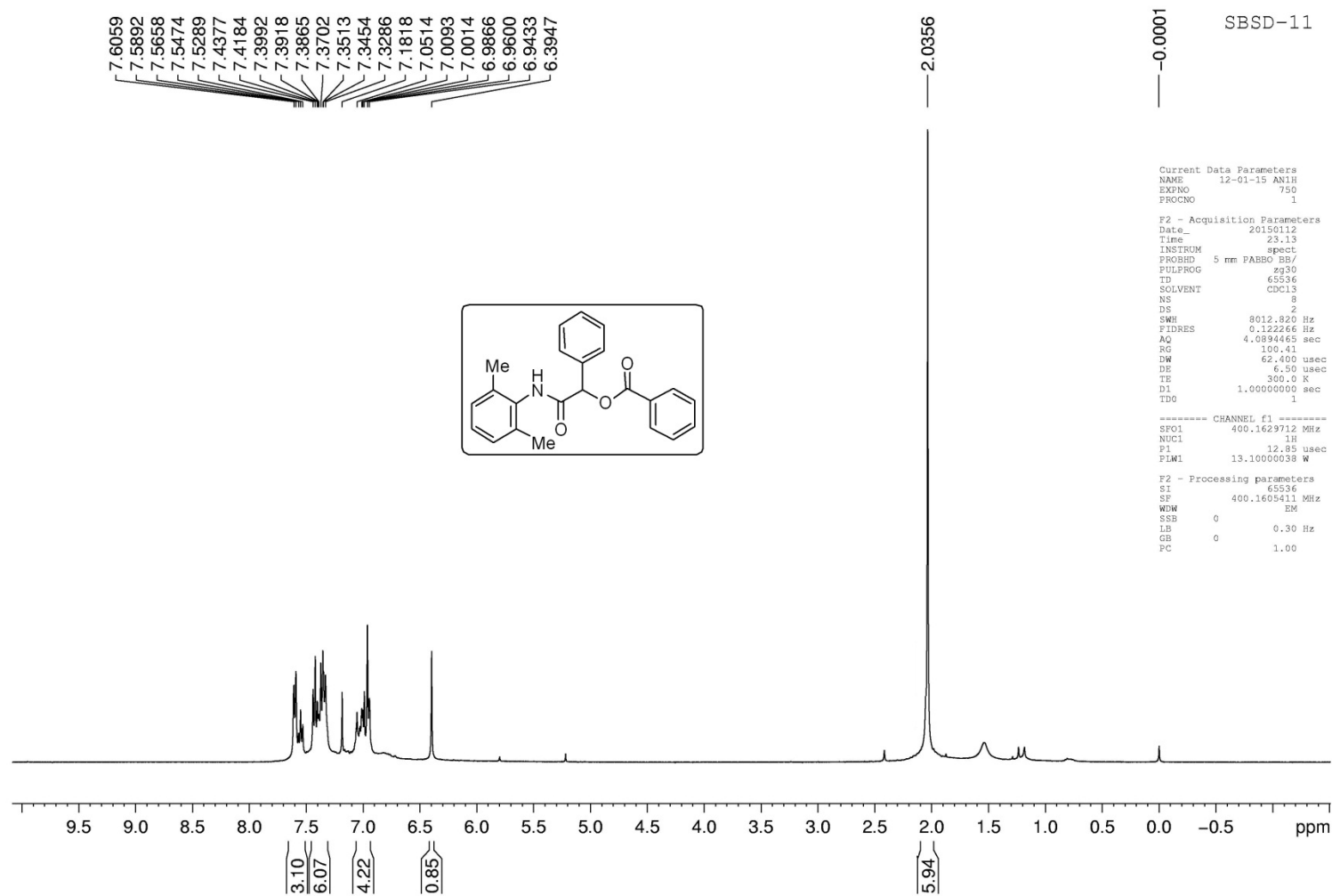
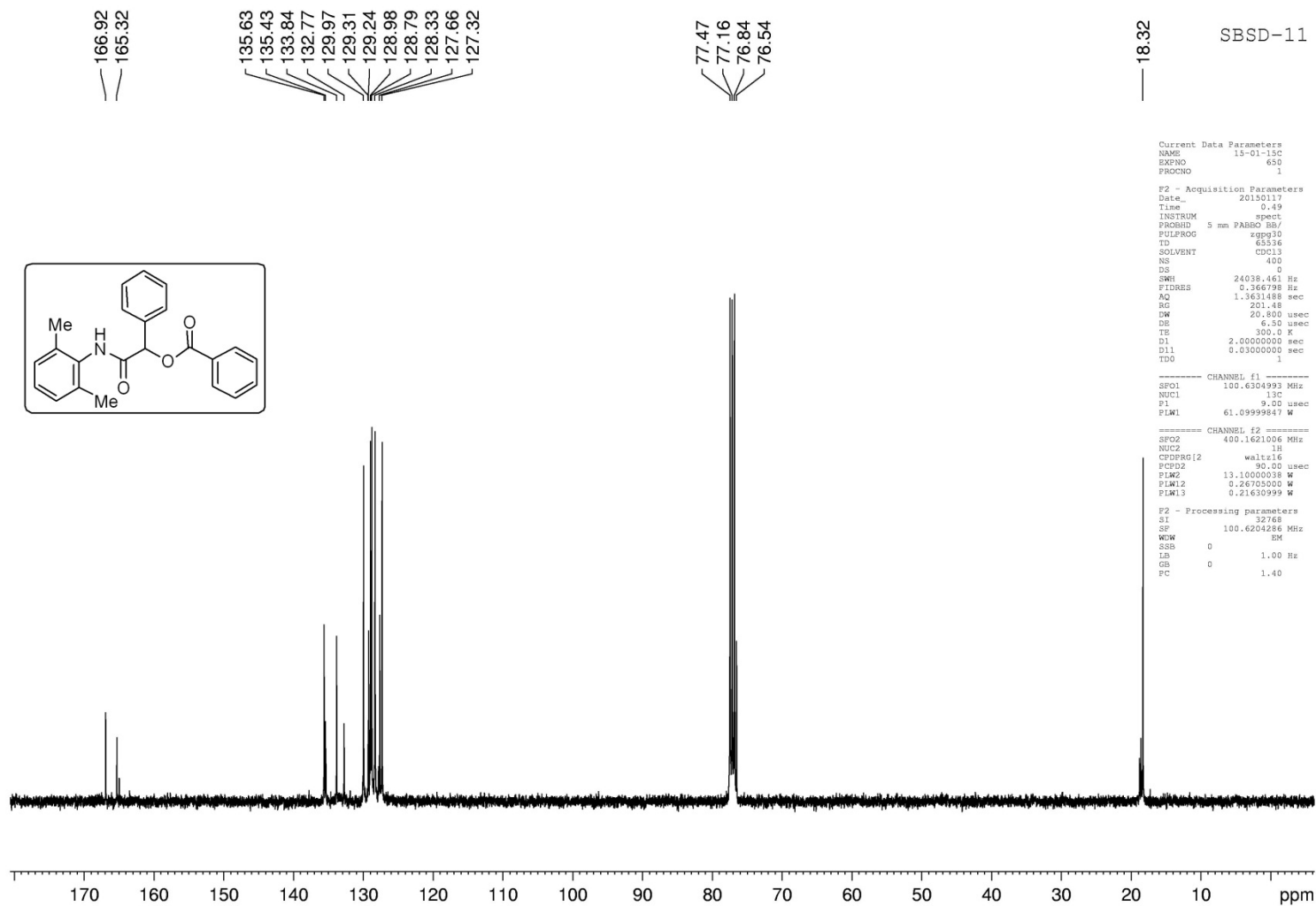
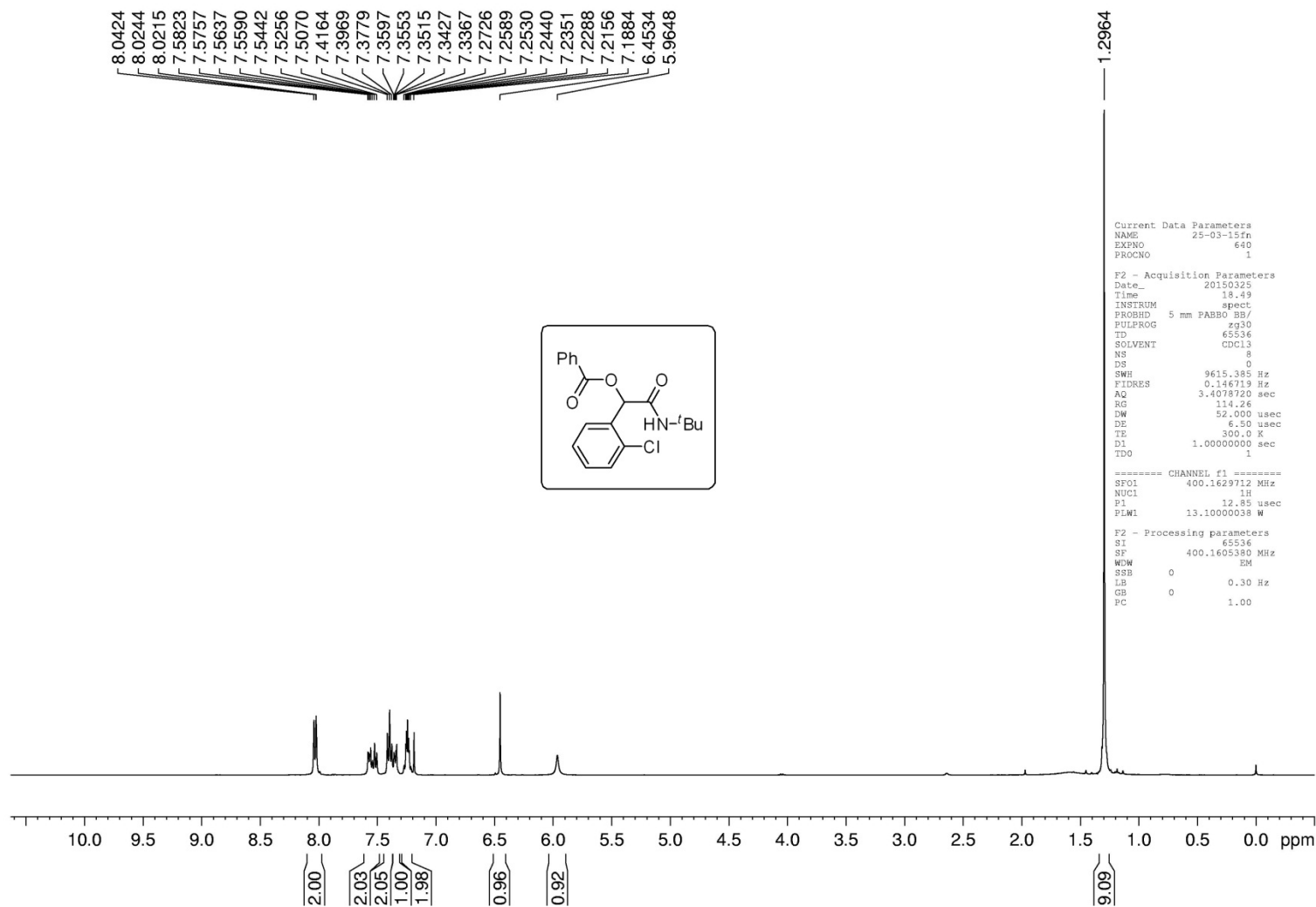


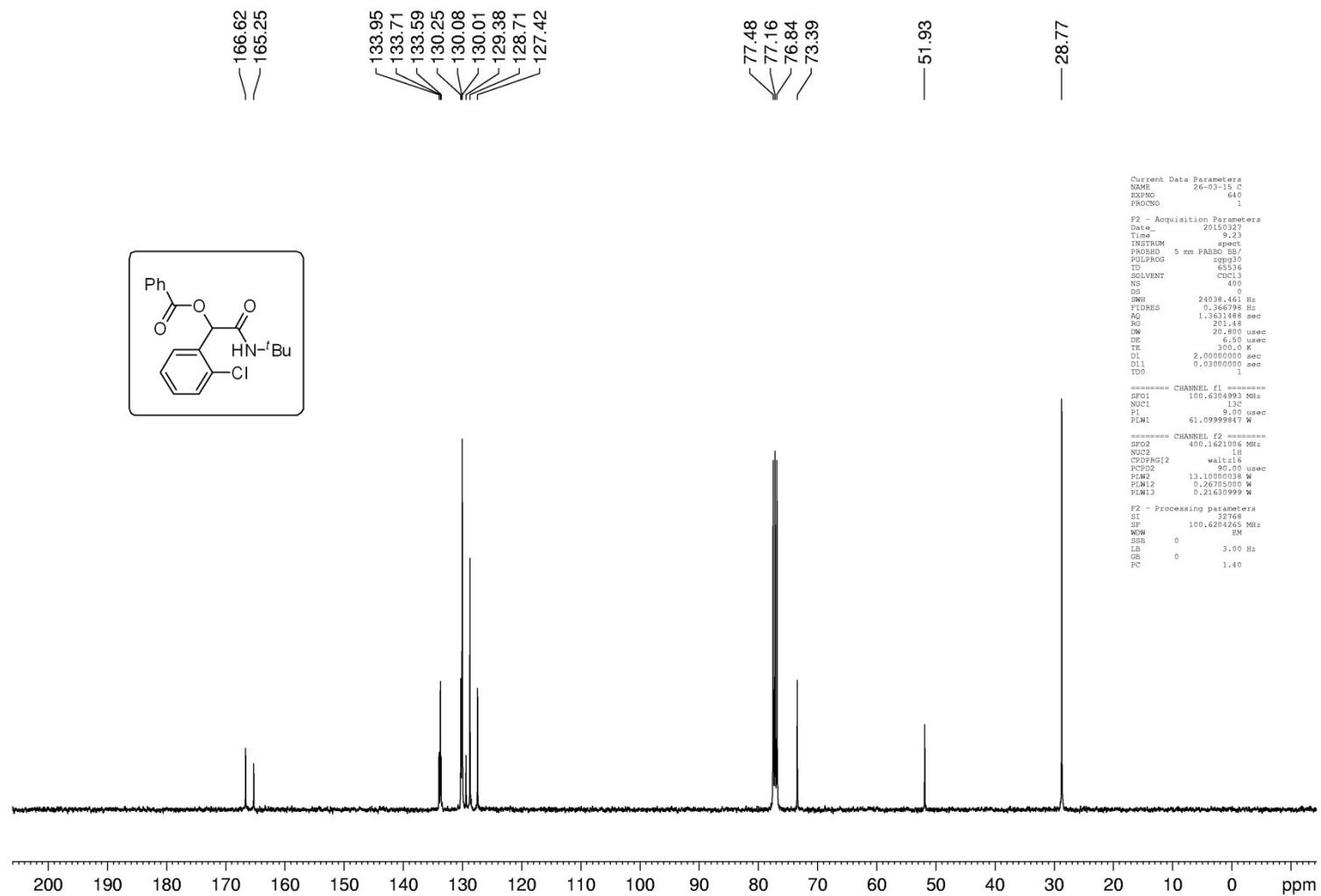
Figure S9. <sup>1</sup>H-NMR spectrum of 2-((2,6-dimethylphenyl)amino)-2-oxo-1-phenylethyl benzoate (4aAe).



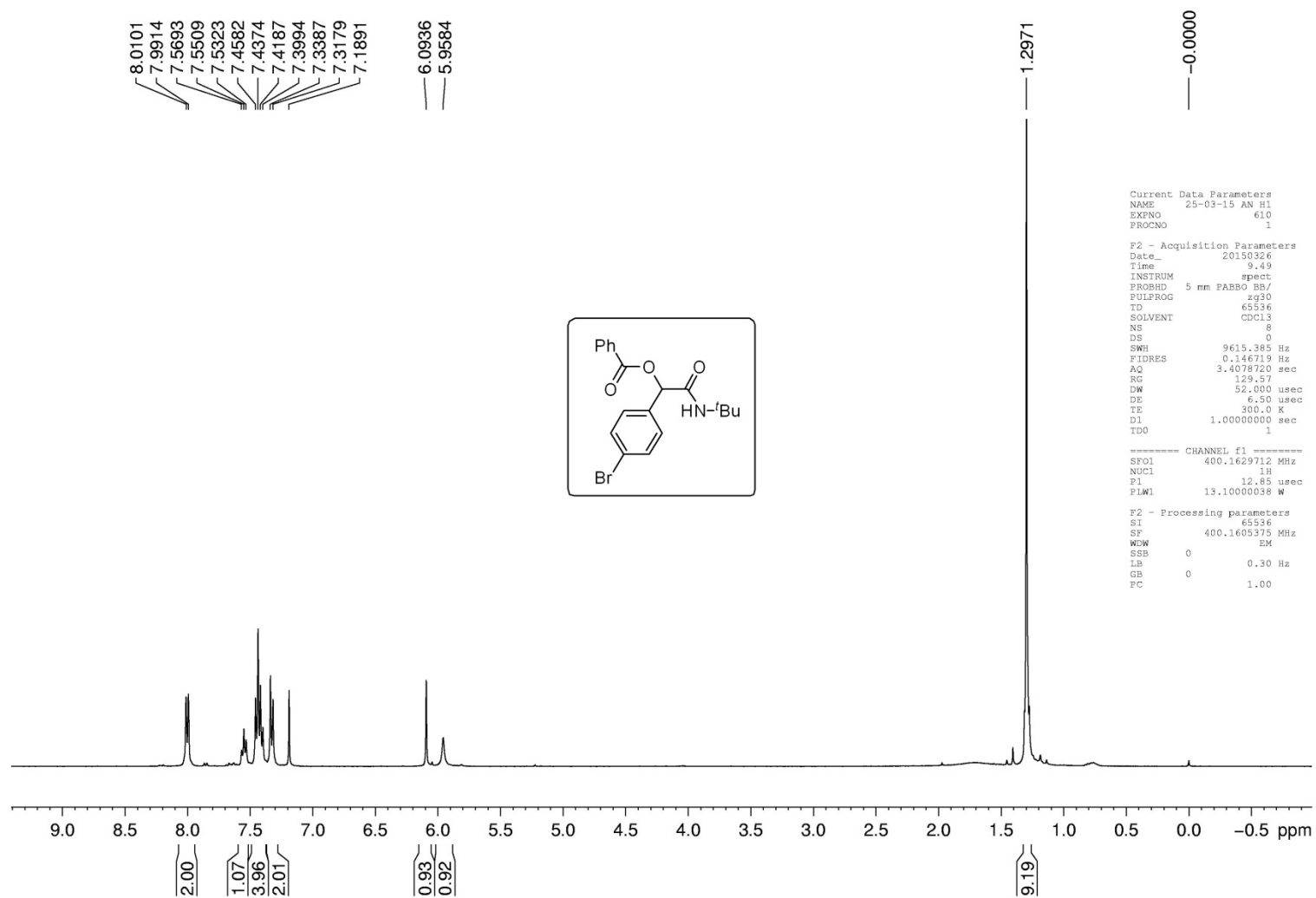
**Figure S10.**  $^{13}\text{C}$ -NMR spectrum of 2-((2,6-dimethylphenyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAe**).



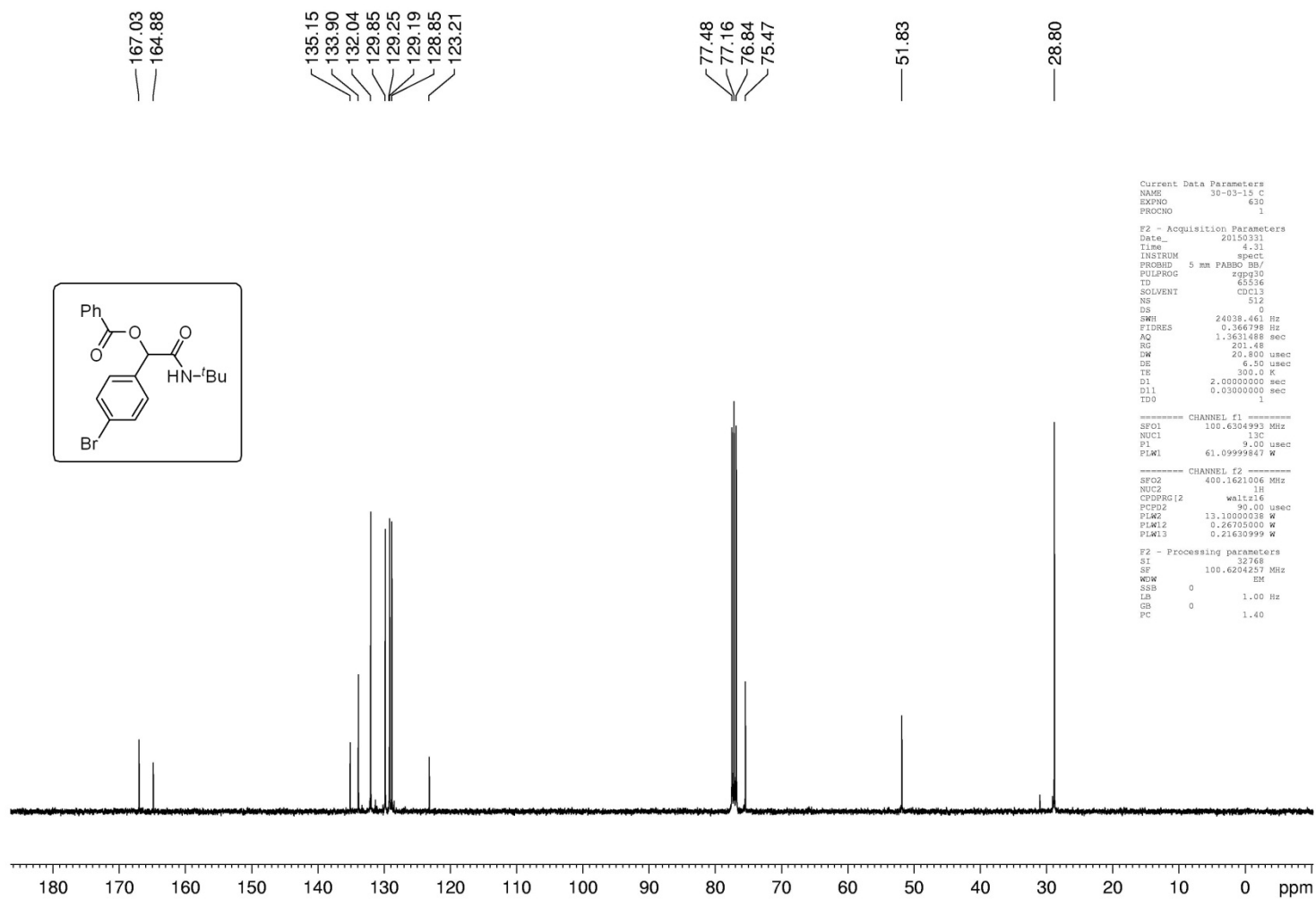
**Figure S11.** <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl benzoate (**4bAa**).



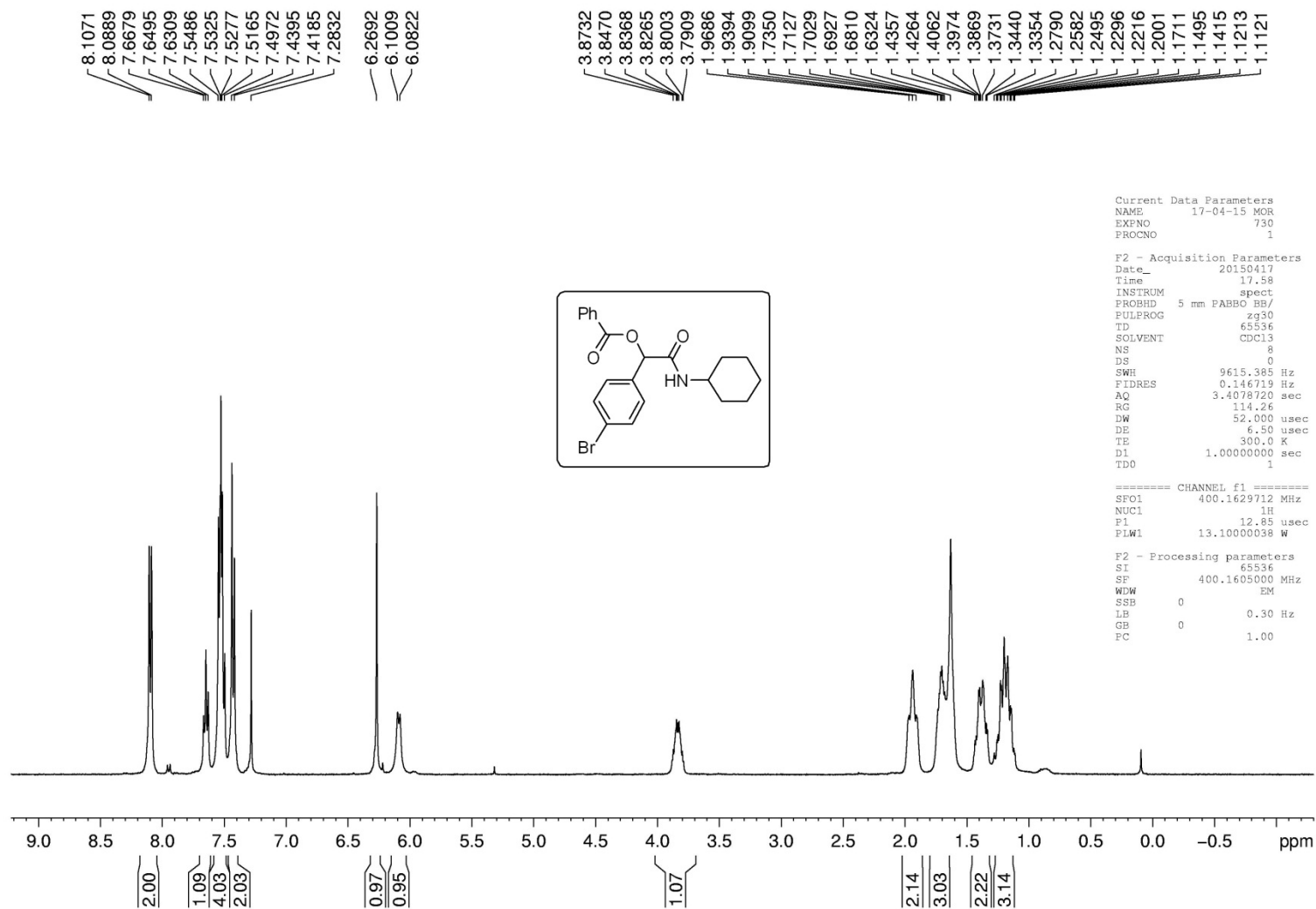
**Figure S12.** <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl benzoate (**4bAa**).



**Figure S13.** <sup>1</sup>H-NMR spectrum of 1-(4-bromophenyl)-2-(tert-butylamino)-2-oxoethyl benzoate (**4cAa**).



**Figure S14.** <sup>13</sup>C-NMR spectrum of 1-(4-bromophenyl)-2-(tert-butylamino)-2-oxoethyl benzoate (**4cAa**).



**Figure S15.**  $^1\text{H-NMR}$  spectrum of 1-(4-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (**4cAb**).



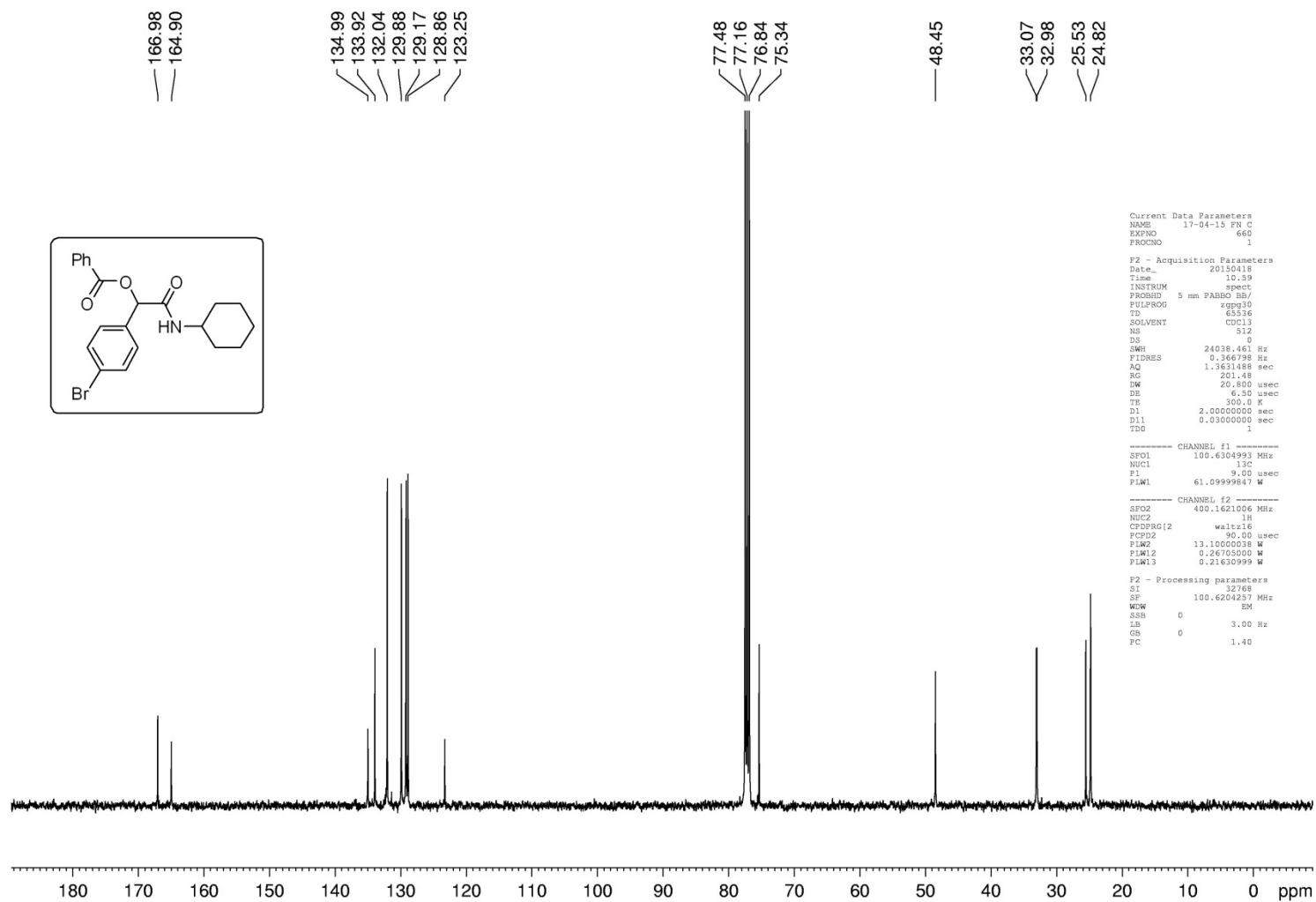
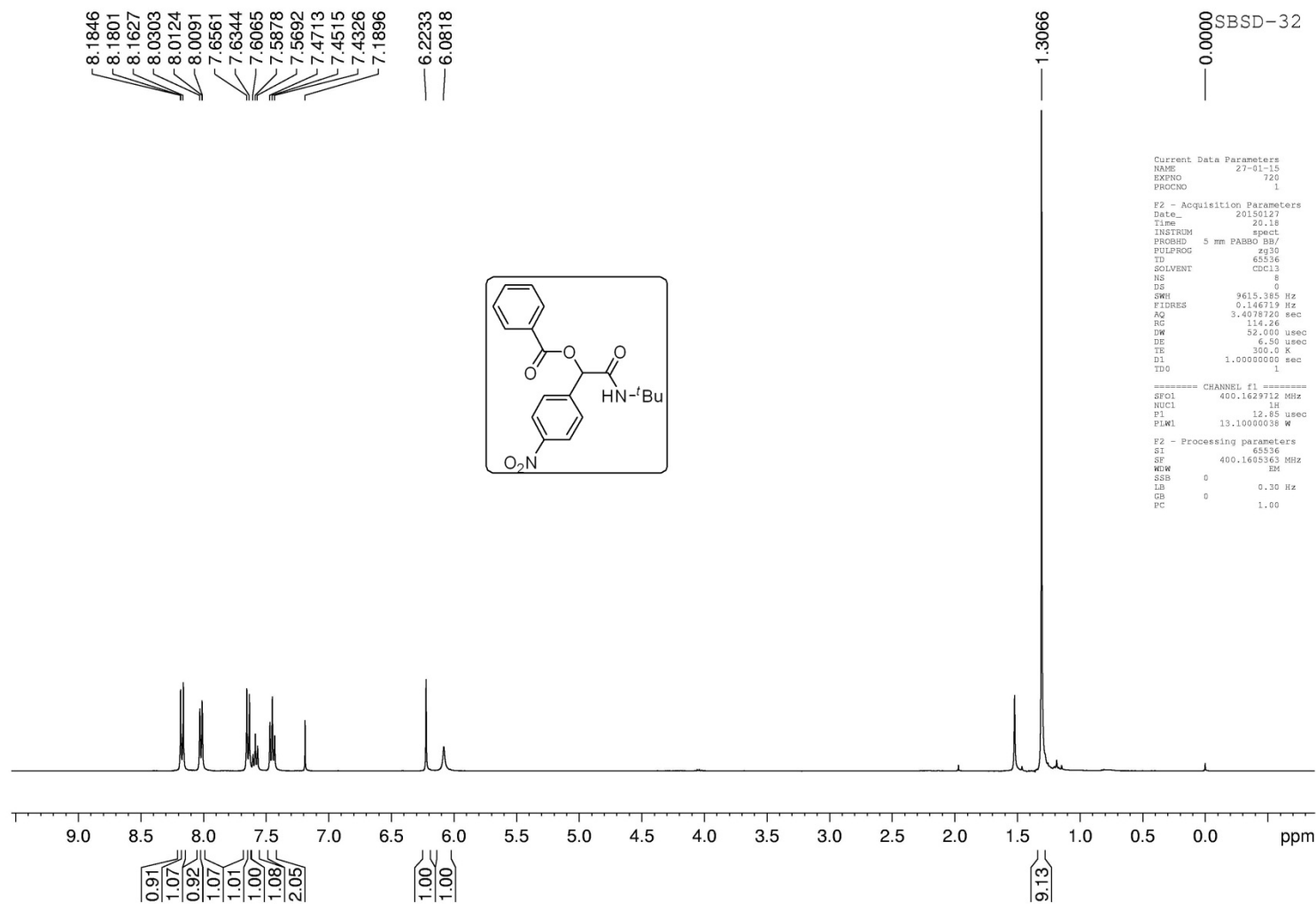


Figure S16. <sup>13</sup>C-NMR spectrum of 1-(4-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (4cAb).



**Figure S17.**  $^1\text{H-NMR}$  spectrum of 2-(*tert*-butylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (**4dAa**).

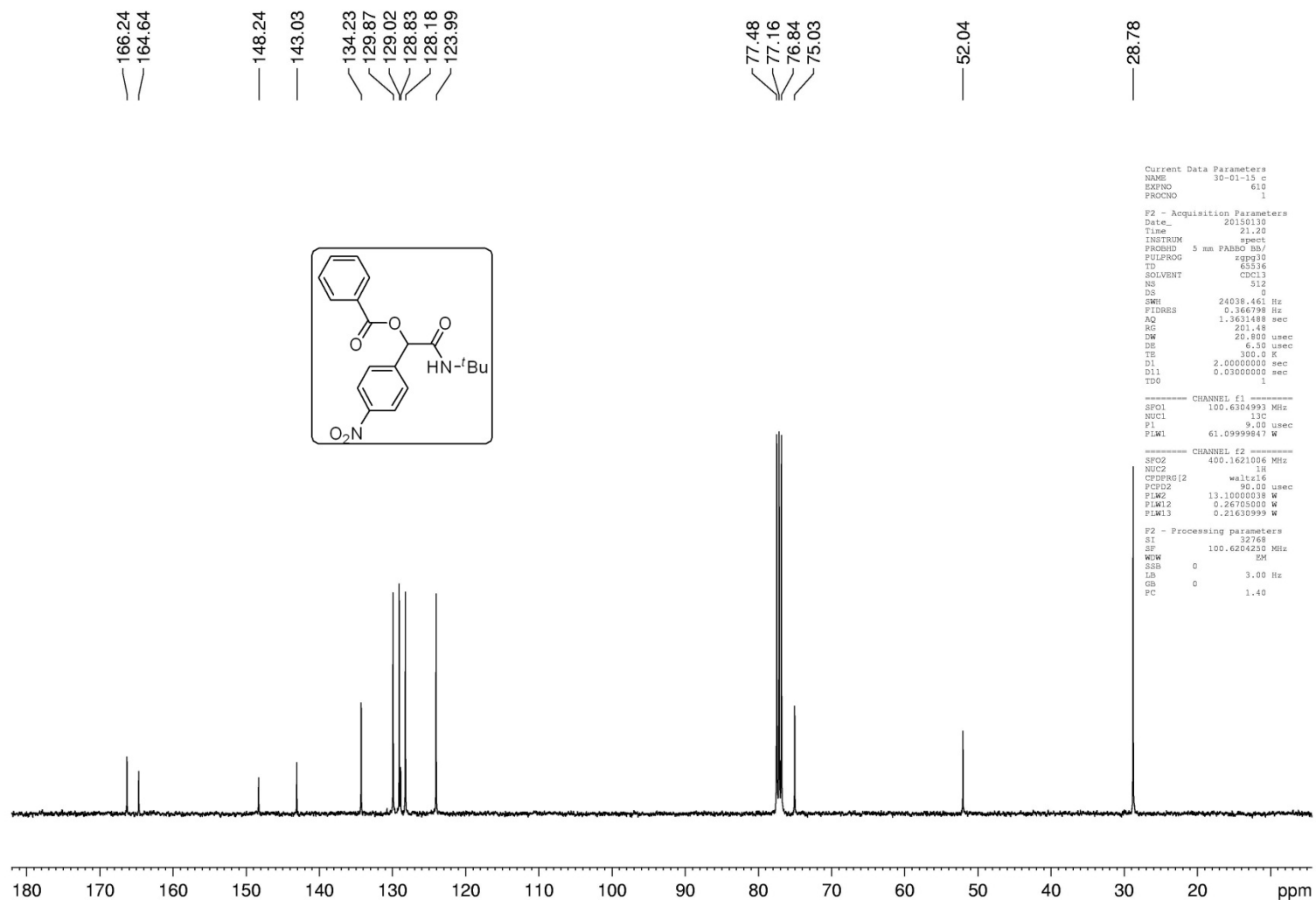
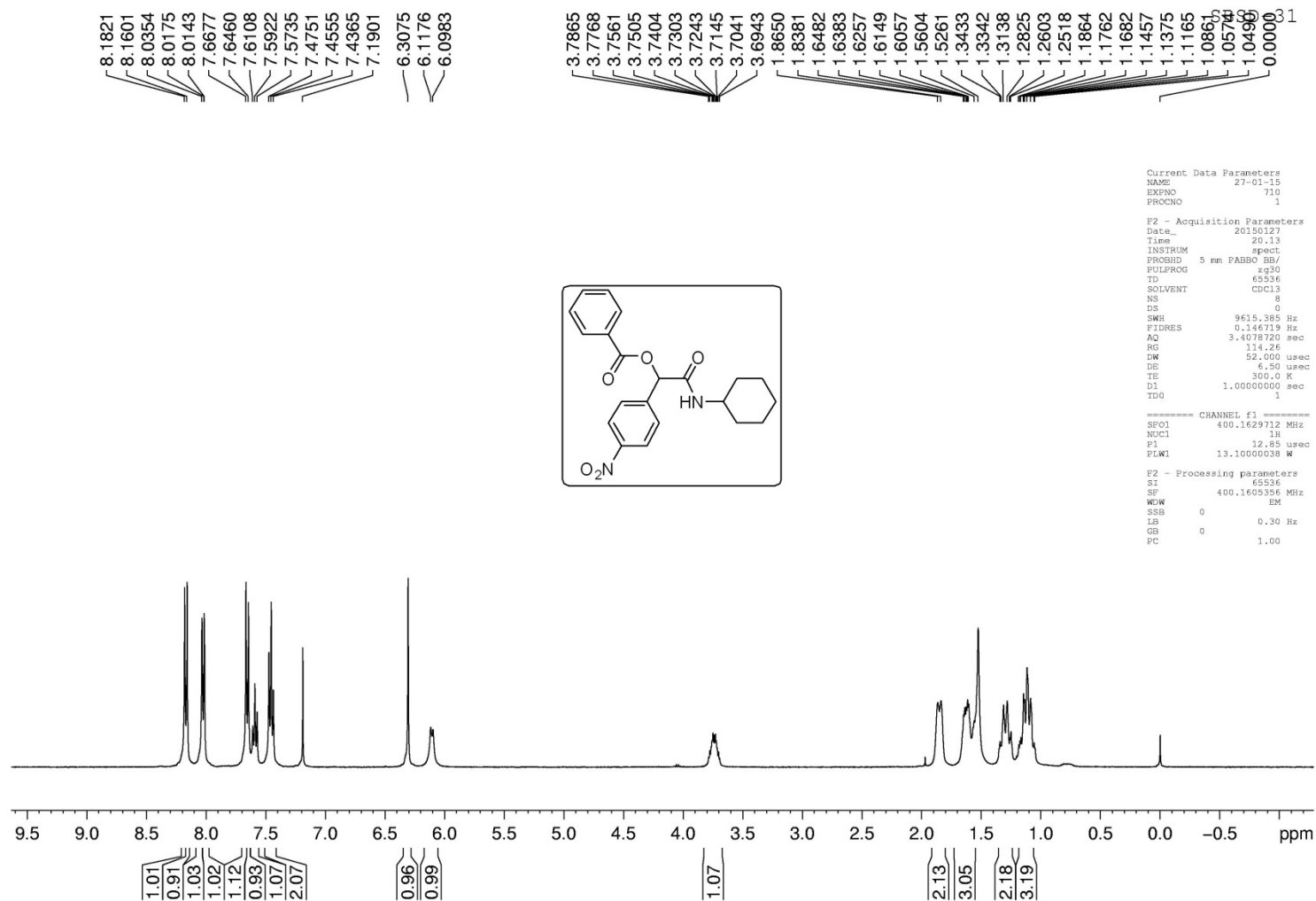


Figure S18.  $^{13}\text{C}$ -NMR spectrum of 2-(*tert*-butylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (4dAa).



**Figure S19.**  $^1\text{H-NMR}$  spectrum of 2-(cyclohexylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (**4dAb**).

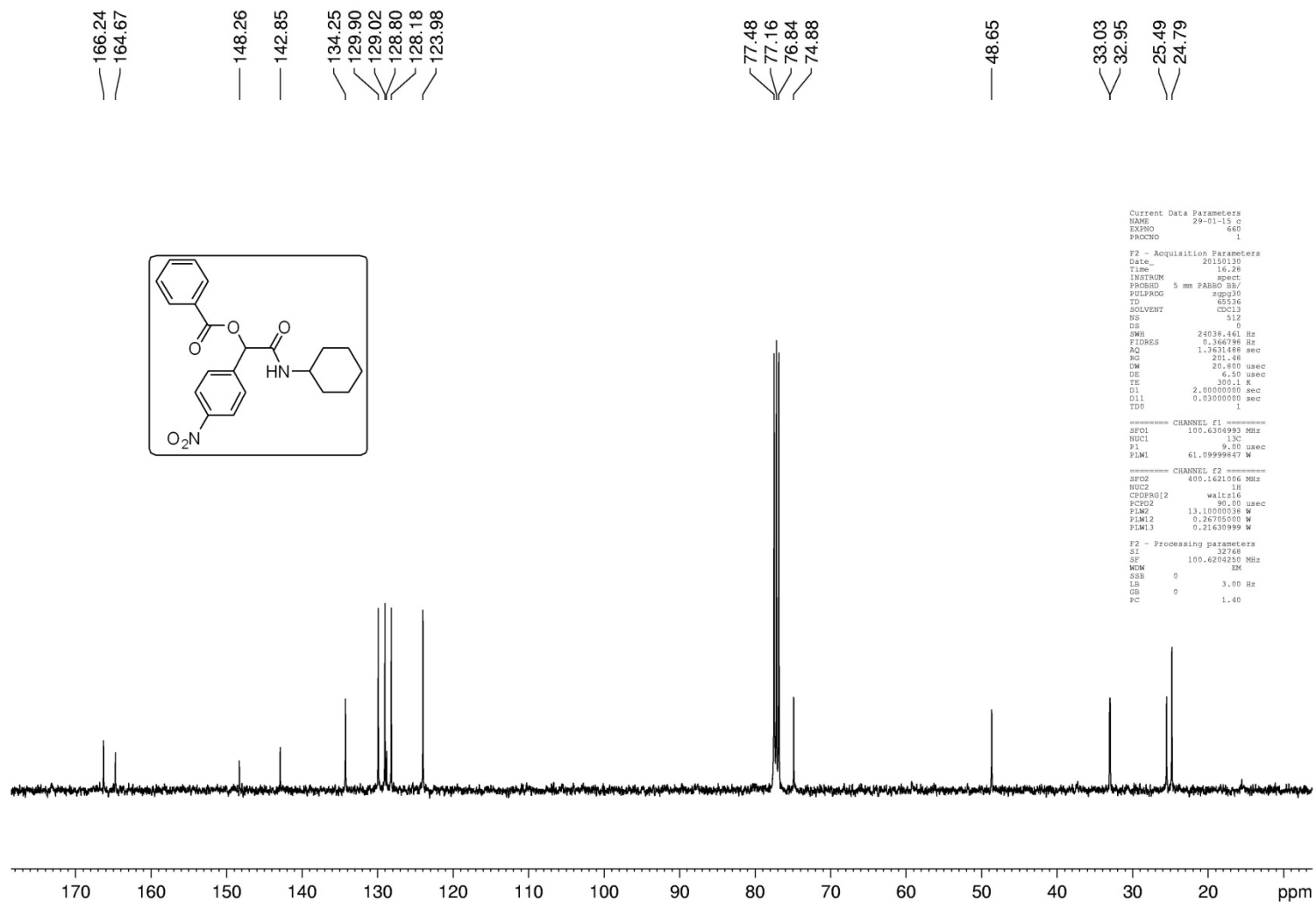
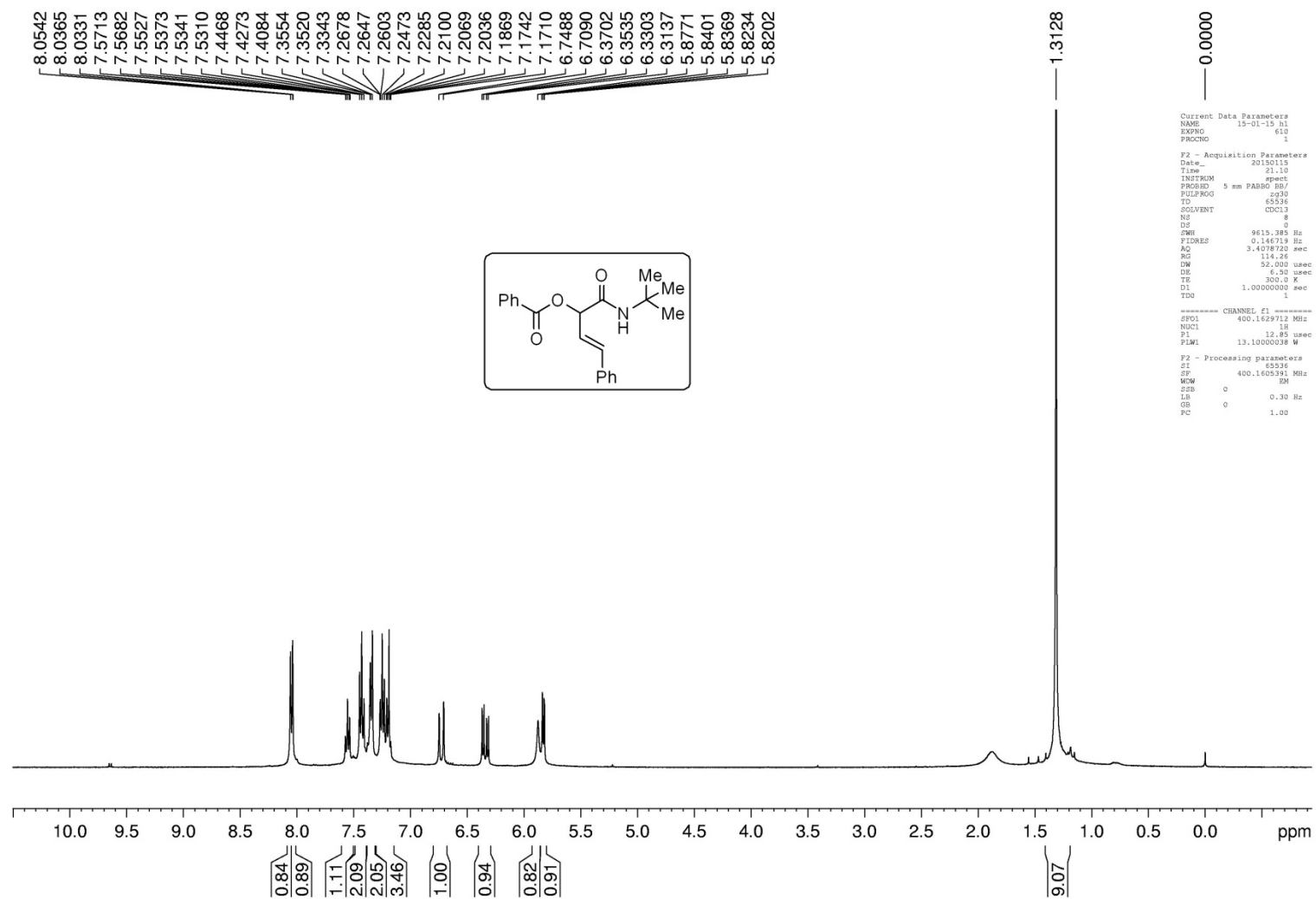


Figure S20. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (**4dAb**).



**Figure S21.**  $^1\text{H-NMR}$  spectrum of (*E*)-1-(*tert*-butylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAa**).

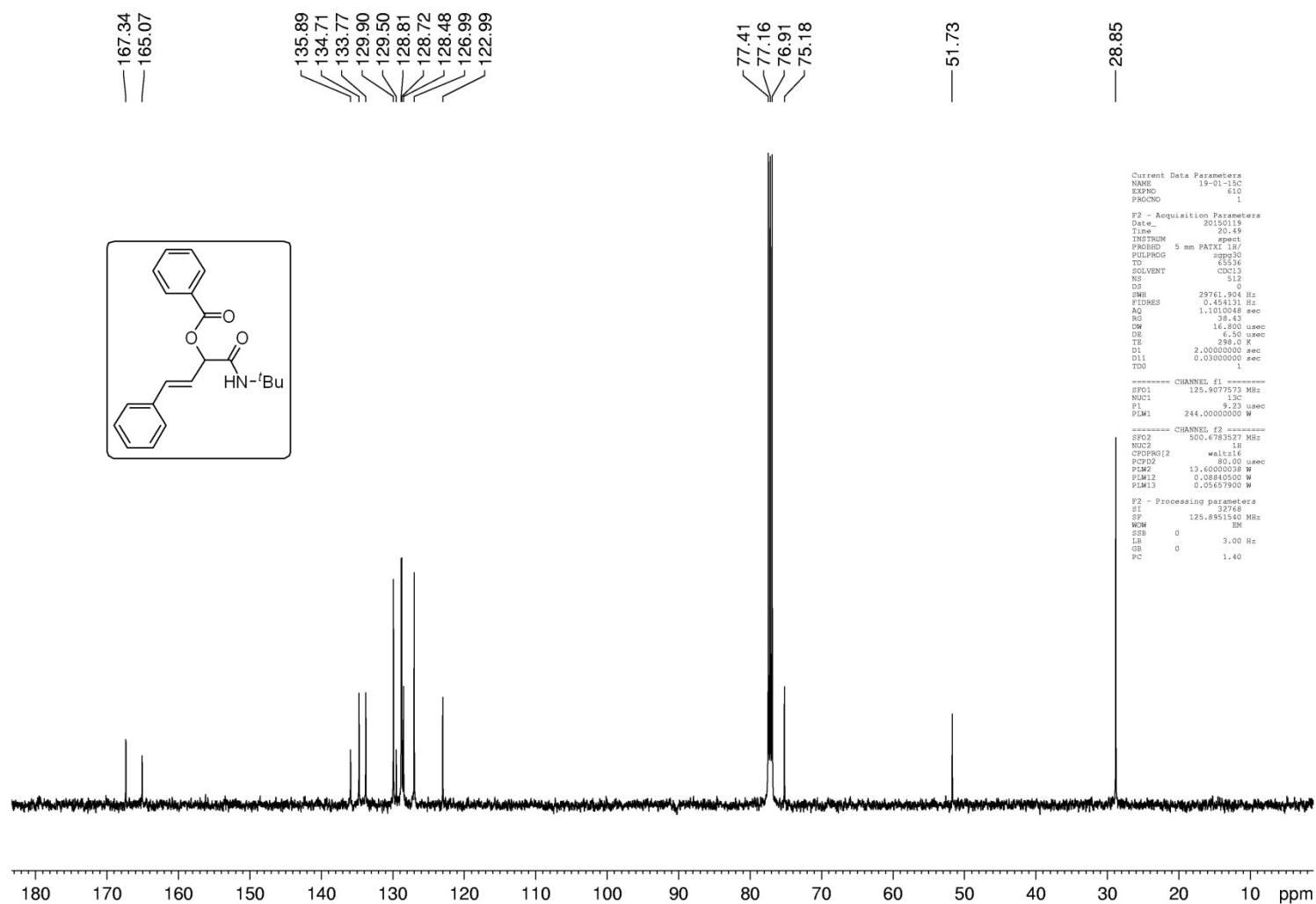


Figure S22. <sup>13</sup>C-NMR spectrum of *(E)*-1-(*tert*-butylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAa**).

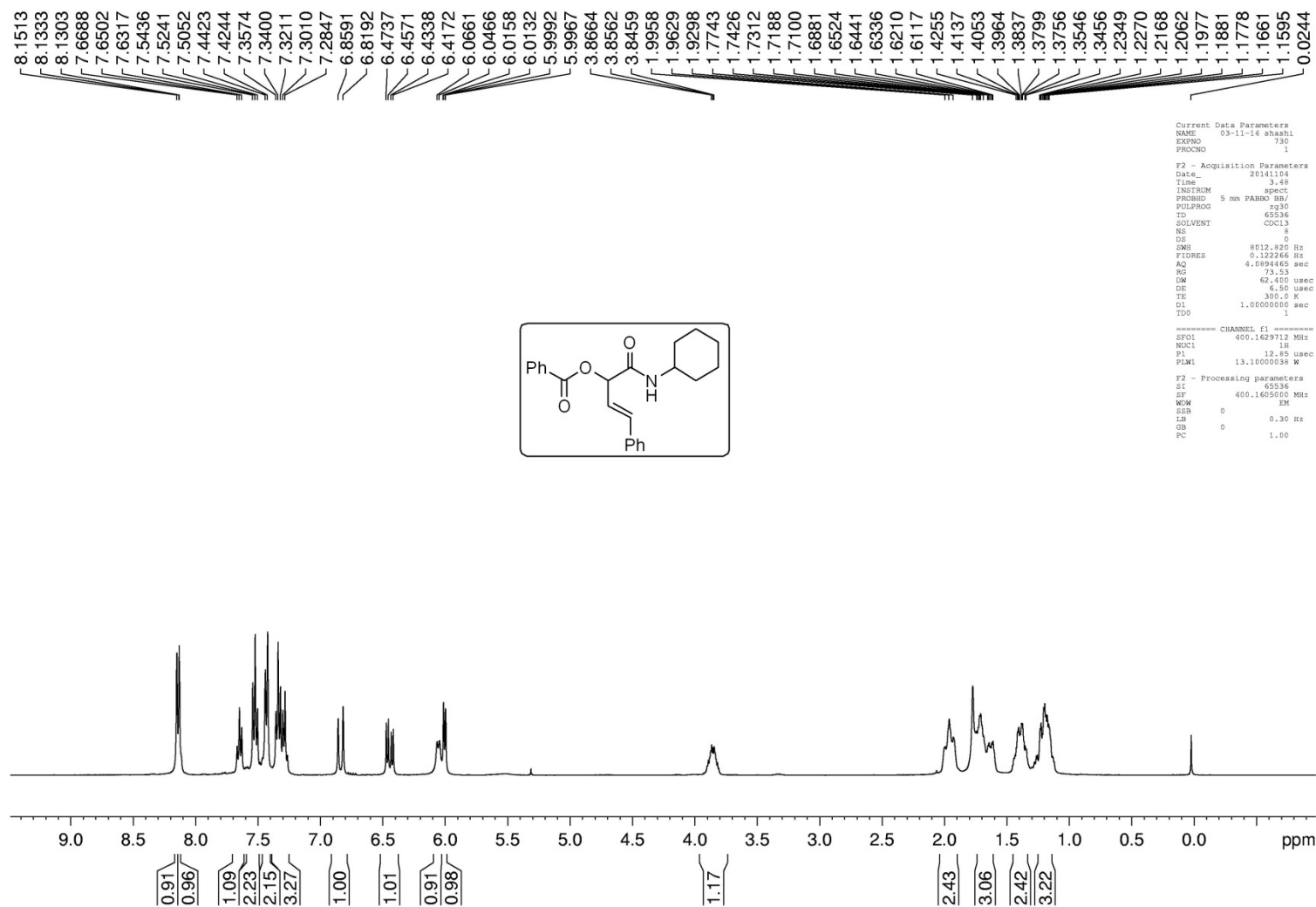
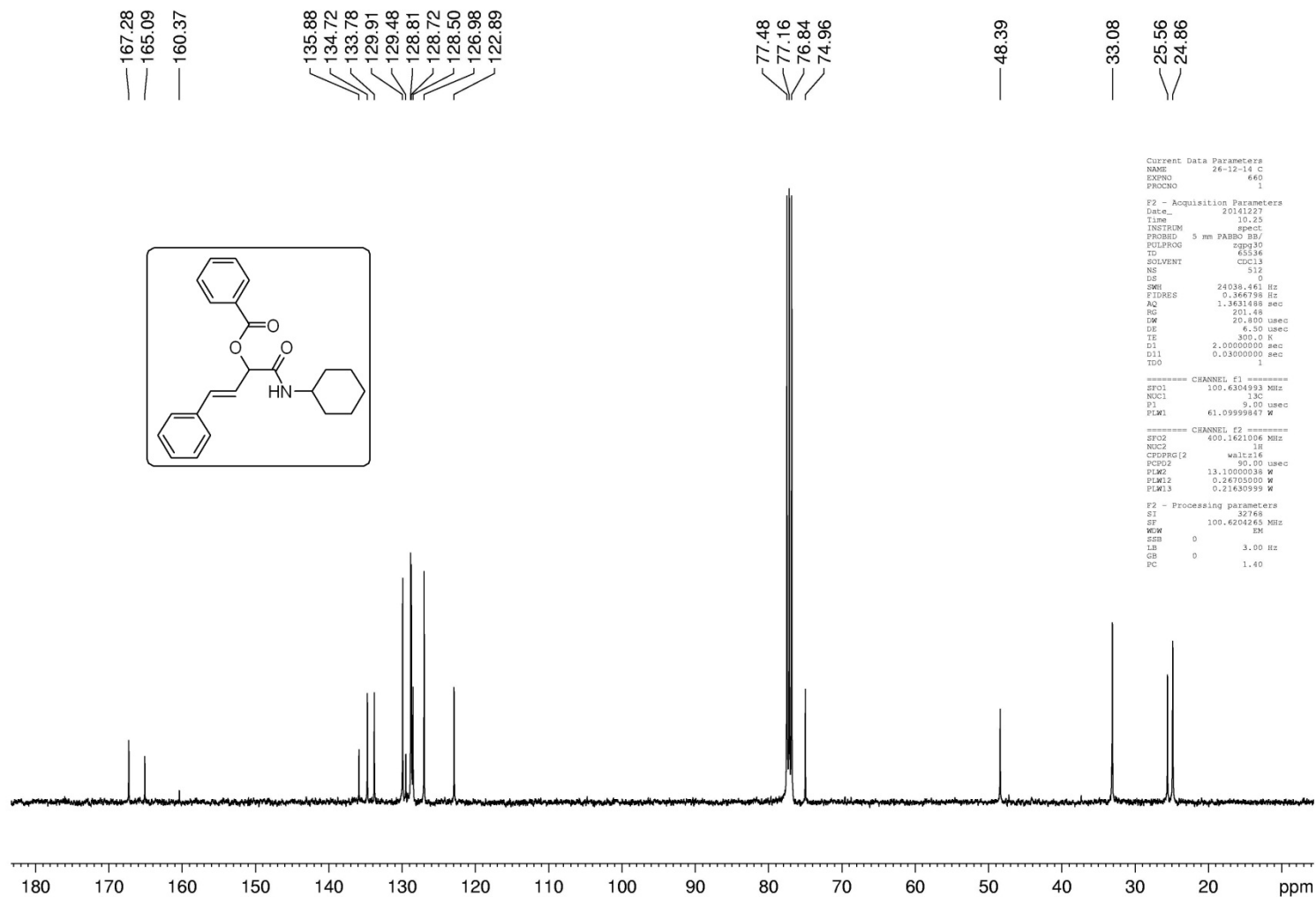


Figure S23. <sup>1</sup>H-NMR spectrum of (E)-1-(cyclohexylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (4eAb).





**Figure S24.** <sup>13</sup>C-NMR spectrum of (*E*)-1-(cyclohexylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAb**).

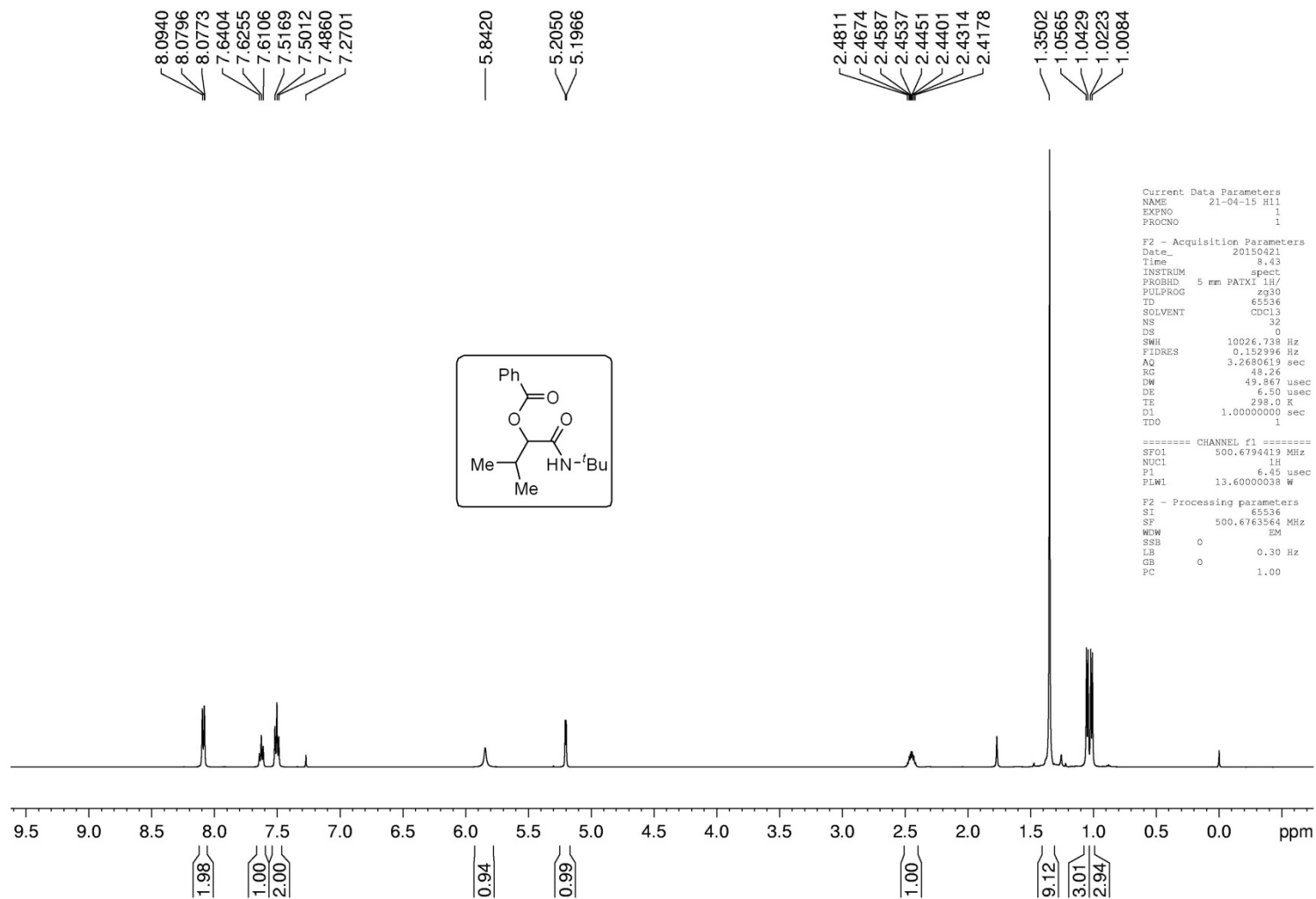


Figure S25. <sup>1</sup>H-NMR spectrum of 1-(*tert*-butylamino)-3-methyl-1-oxobutan-2-yl benzoate (**4fAa**).

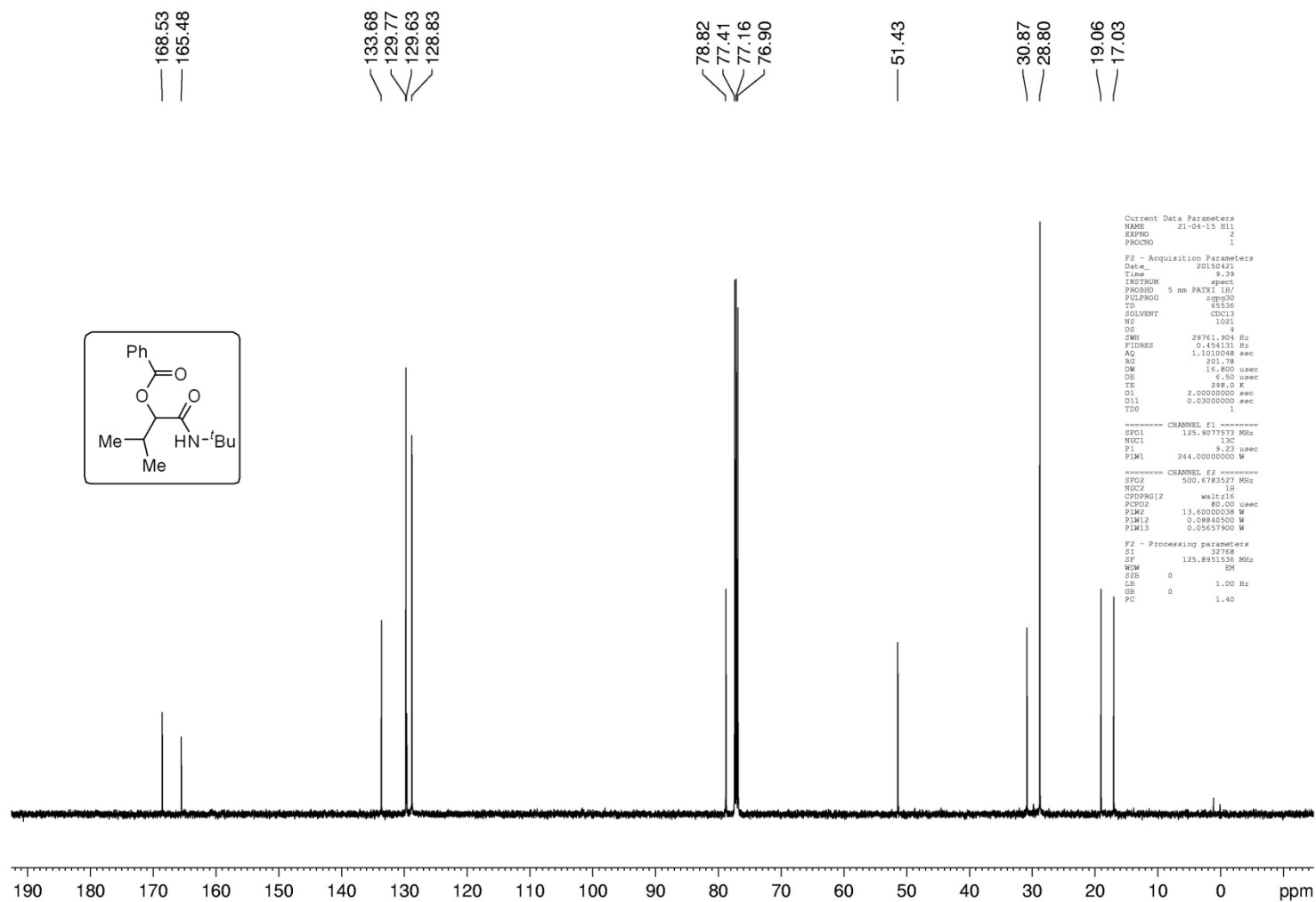


Figure S26.  $^{13}\text{C}$ -NMR spectrum of 1-(*tert*-butylamino)-3-methyl-1-oxobutan-2-yl benzoate (4fAa).

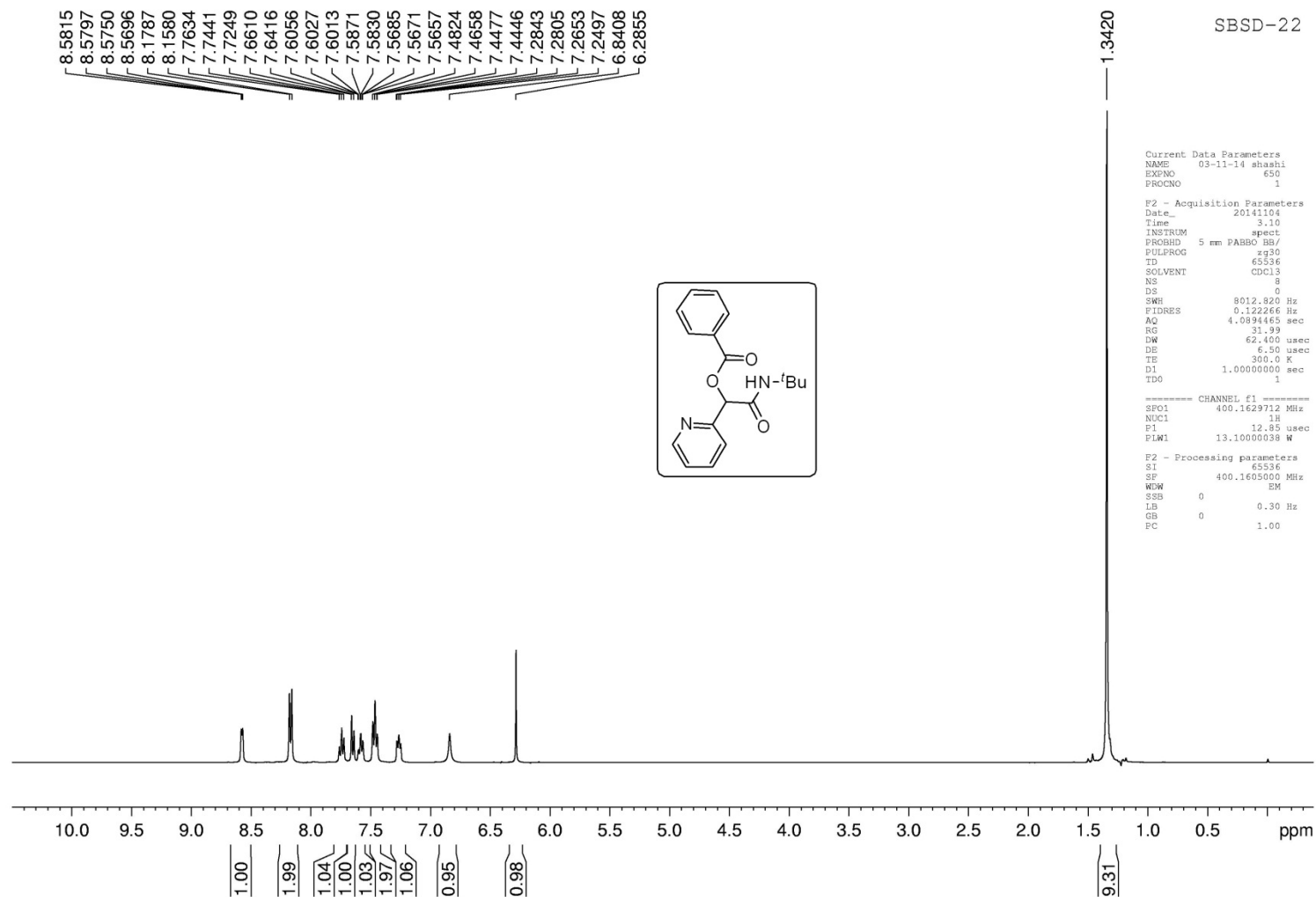


Figure S27. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAa**).

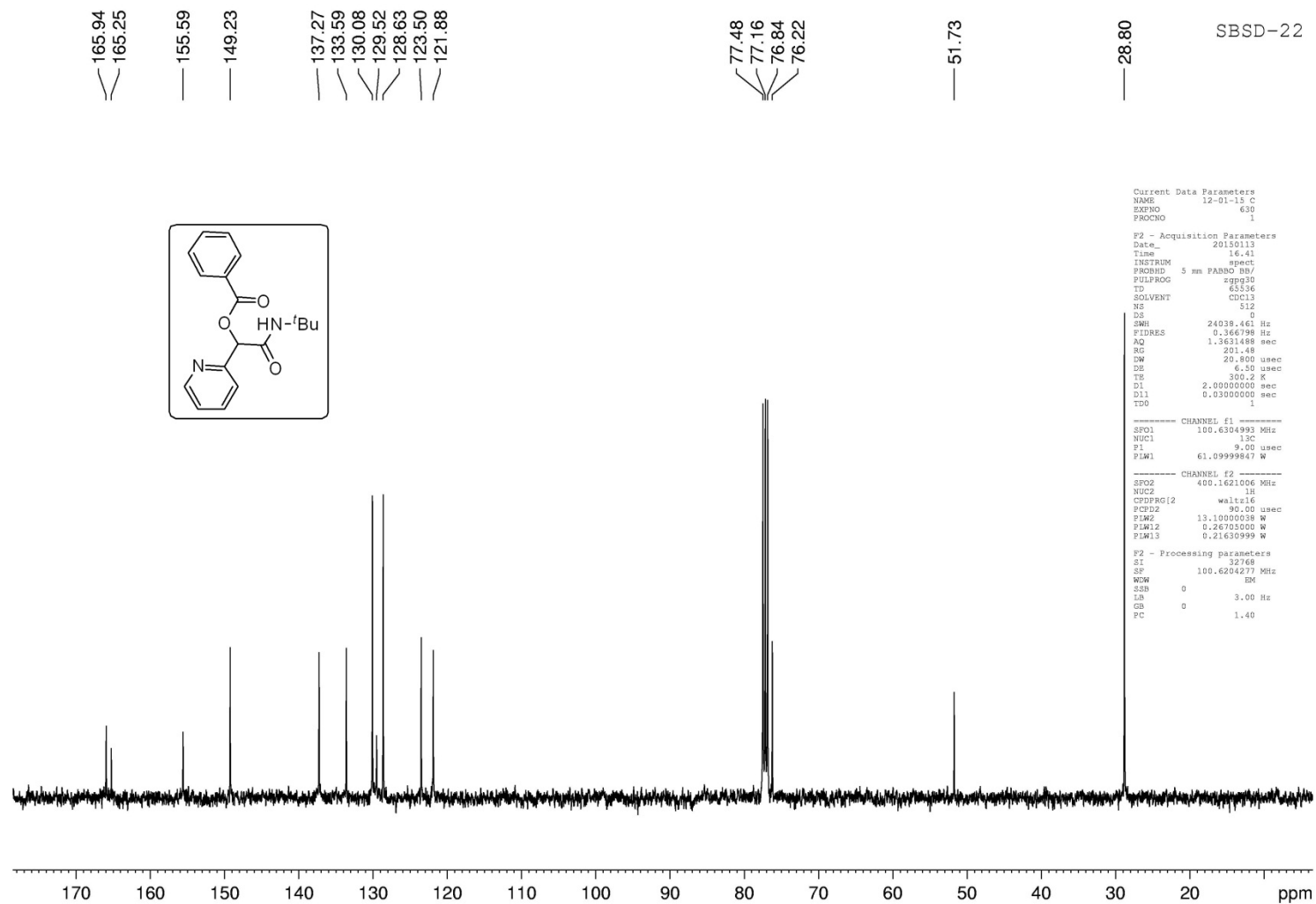
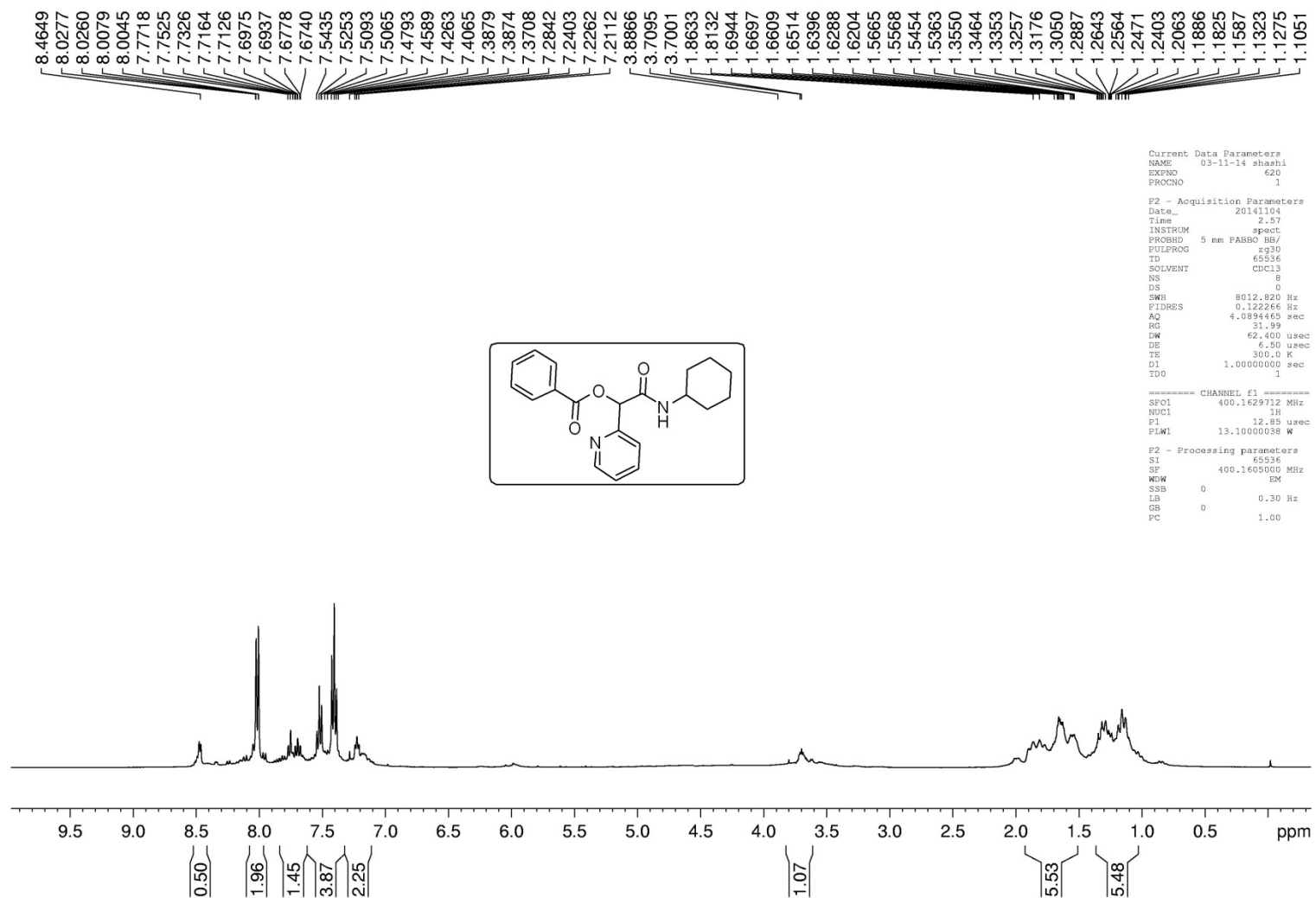


Figure S28.  $^{13}\text{C}$ -NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAa**).



**Figure S29.**  $^1\text{H-NMR}$  spectrum of 2-(cyclohexylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAb**).

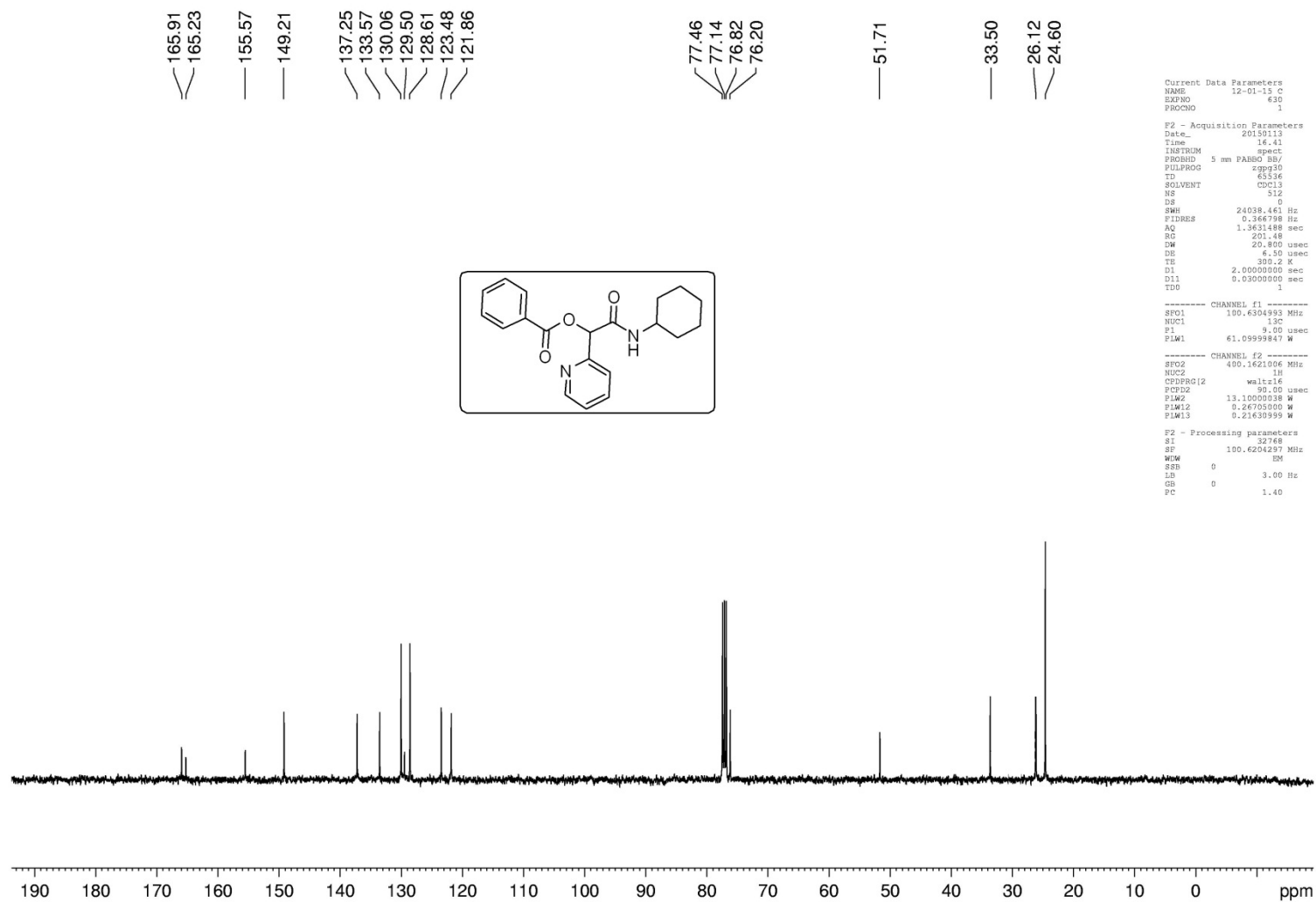
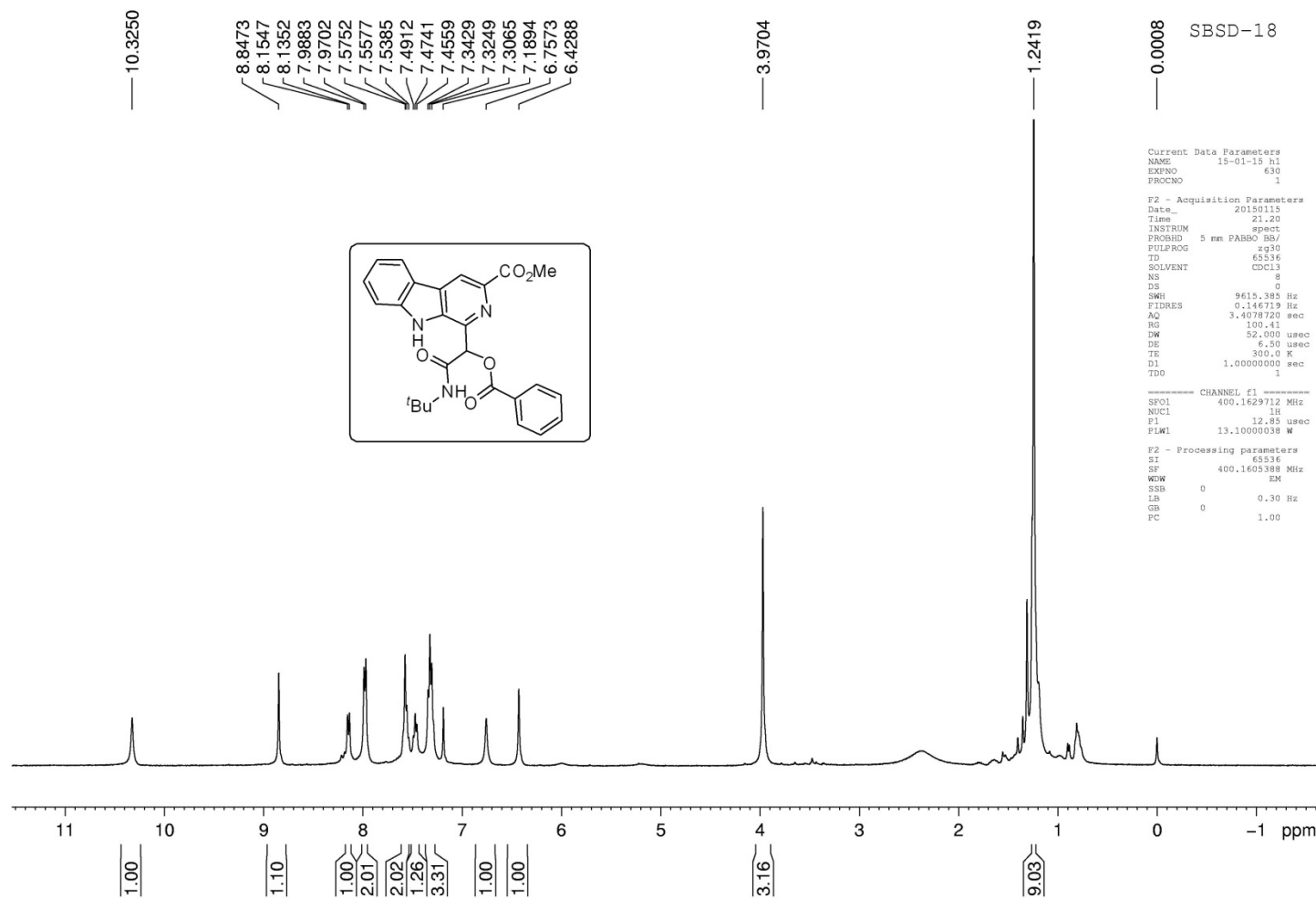
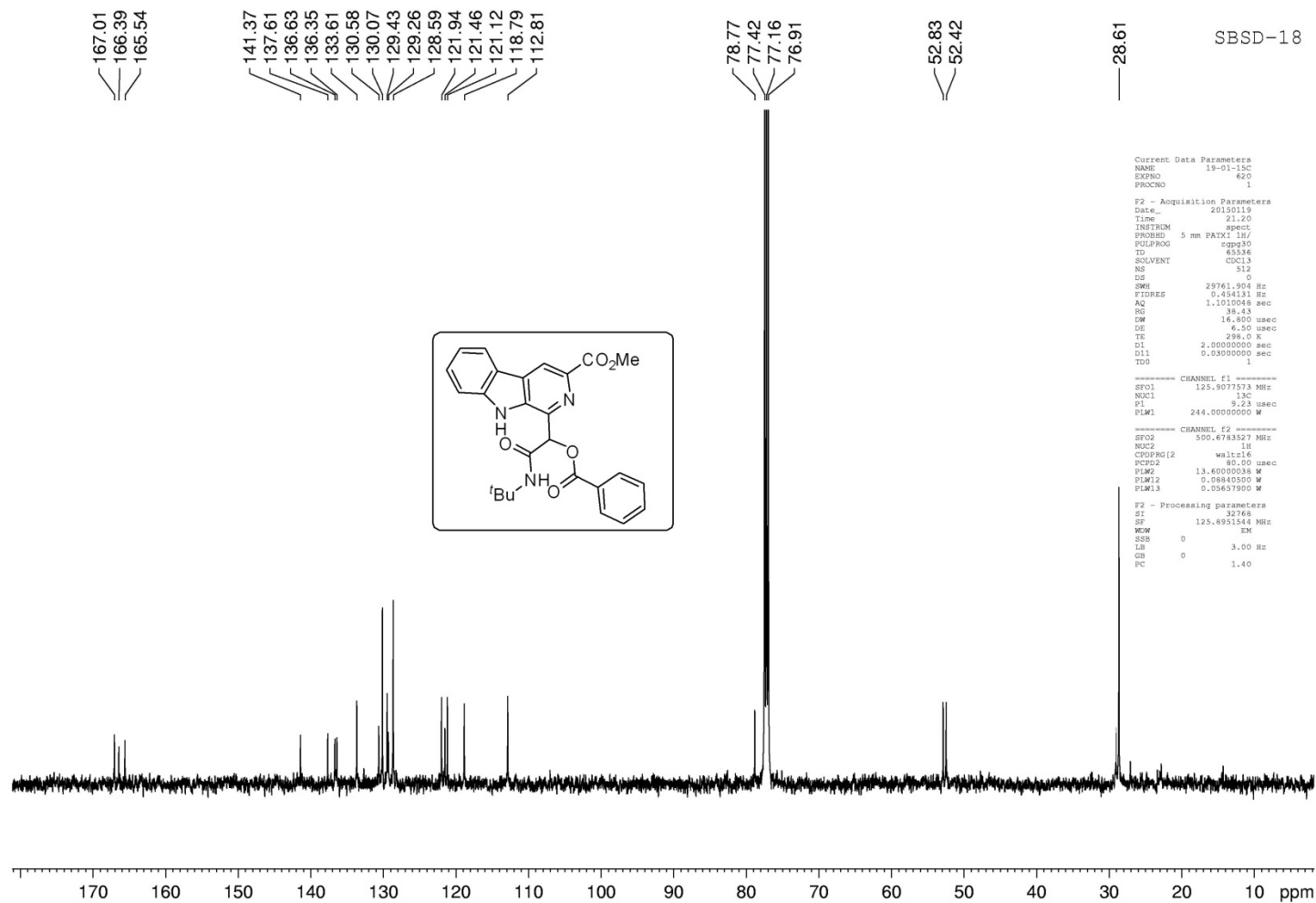


Figure S30.  $^{13}\text{C}$ -NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAb**).

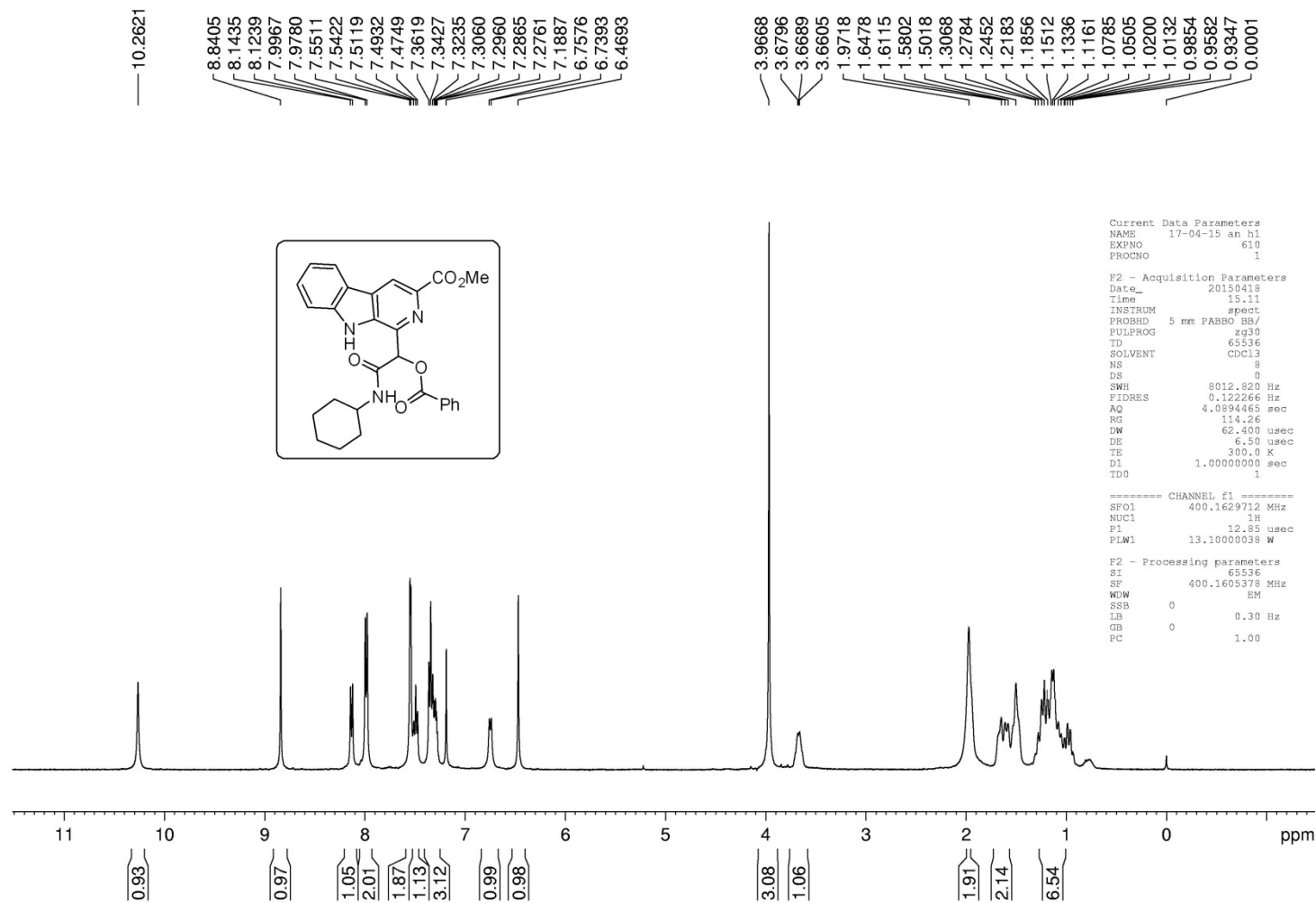


**Figure S31.**  $^1\text{H-NMR}$  spectrum of methyl 1-(1-(benzoyloxy)-2-(*tert*-butylamino)-2-oxoethyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate (4hAa).

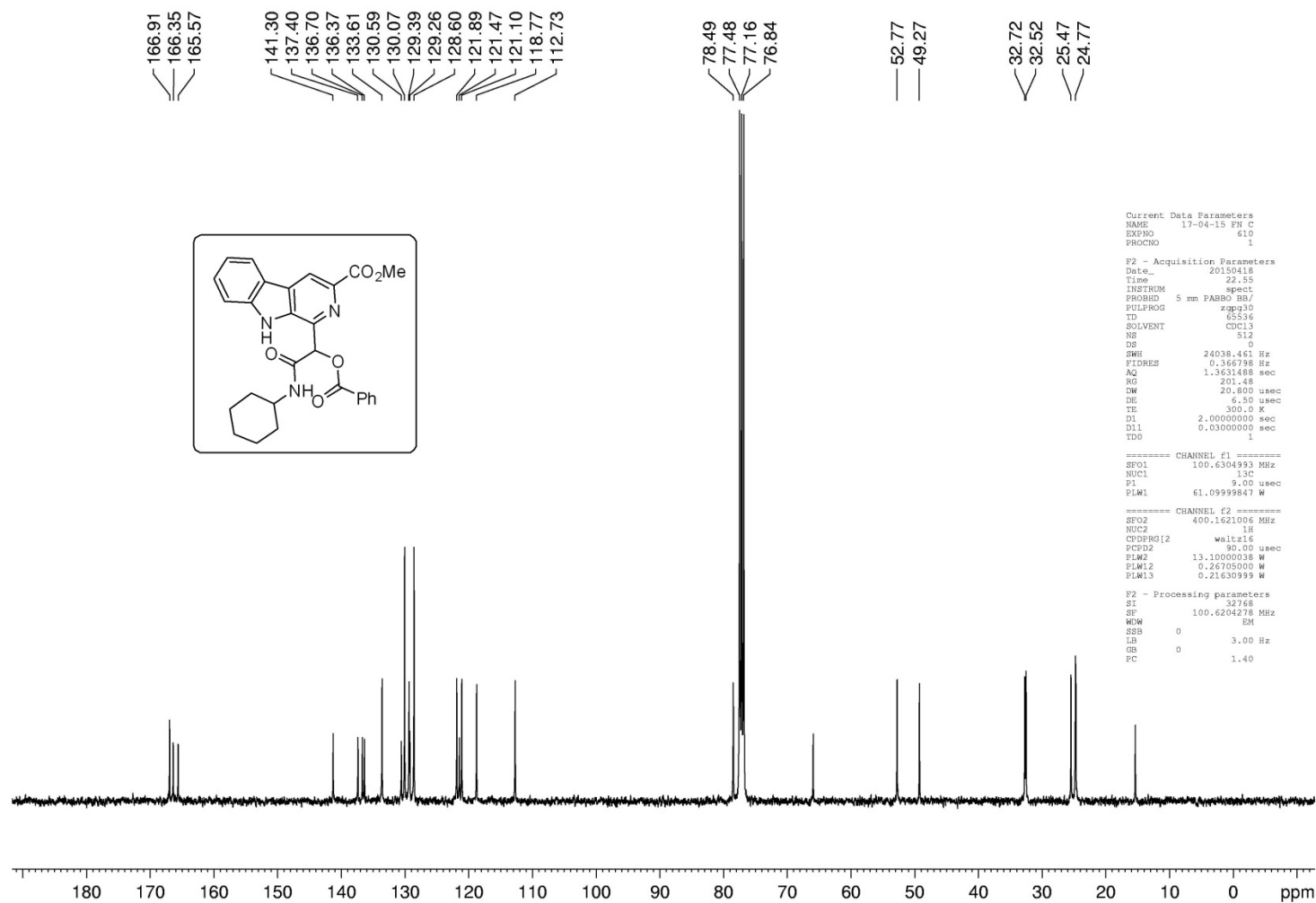




**Figure S32.** <sup>13</sup>C-NMR spectrum of methyl 1-(1-(benzoyloxy)-2-(tert-butylamino)-2-oxoethyl)-9H-pyrido[3,4-b]indole-3-carboxylate (4hAa).



**Figure S33.** <sup>1</sup>H-NMR spectrum of methyl 1-(1-(benzoyloxy)-2-(cyclohexylamino)-2-oxoethyl)-9H-pyrido[3,4-b]indole-3-carboxylate (4hAb).



**Figure S34.** <sup>13</sup>C-NMR spectrum of methyl 1-(1-(benzoyloxy)-2-(cyclohexylamino)-2-oxoethyl)-9H-pyrido[3,4-b]indole-3-carboxylate (4hAb).

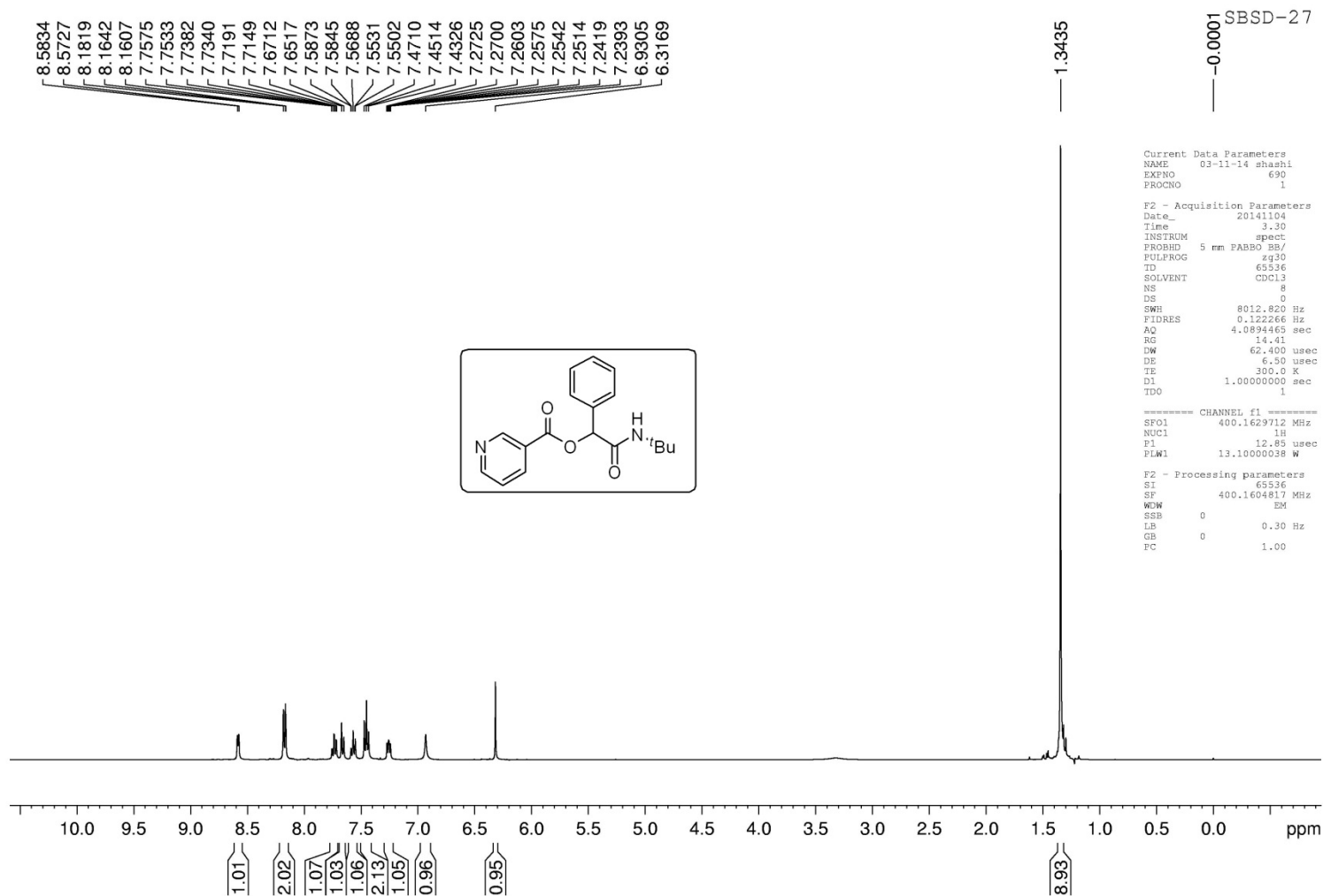


Figure S35. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl nicotinate (**4aBa**).

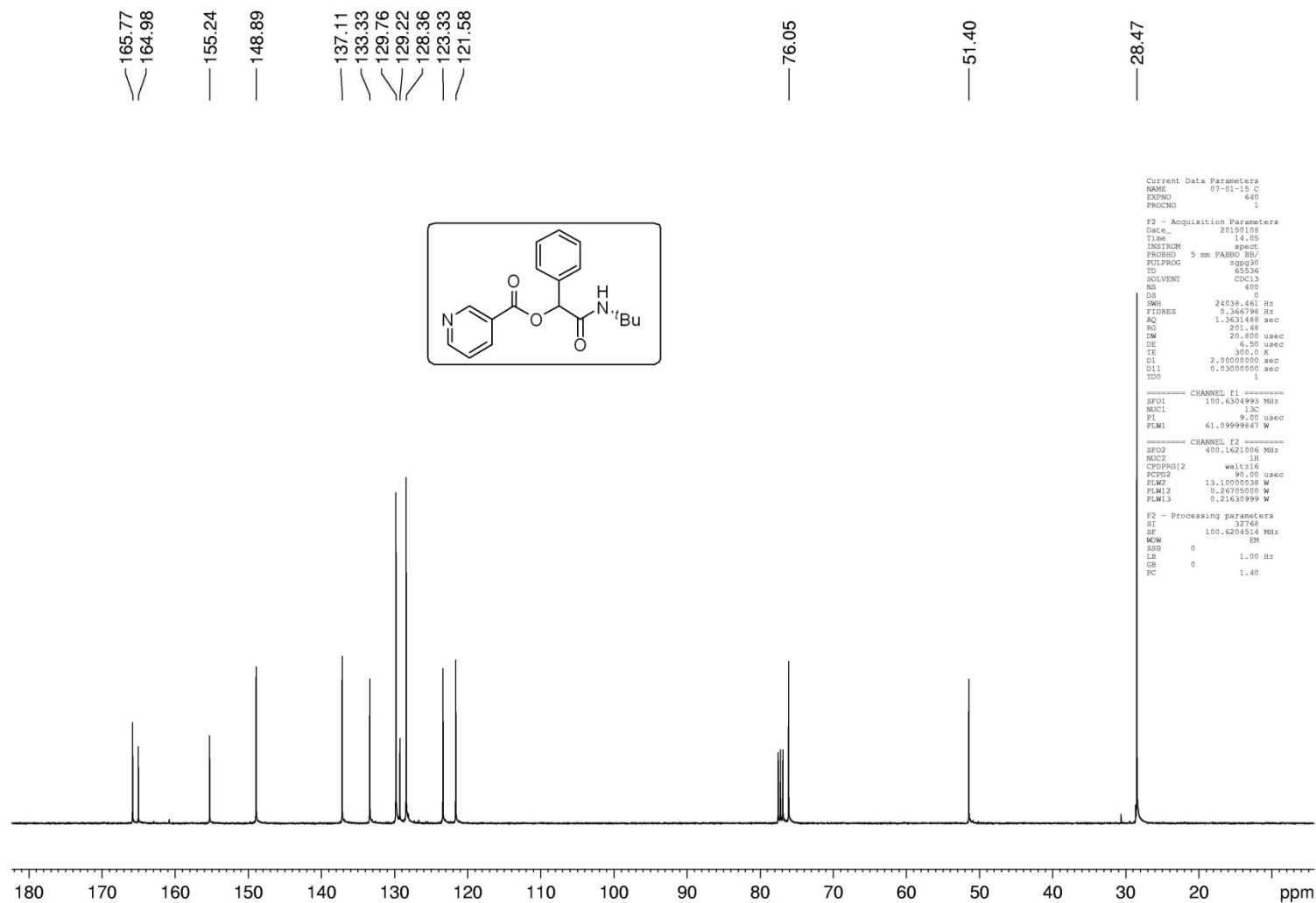
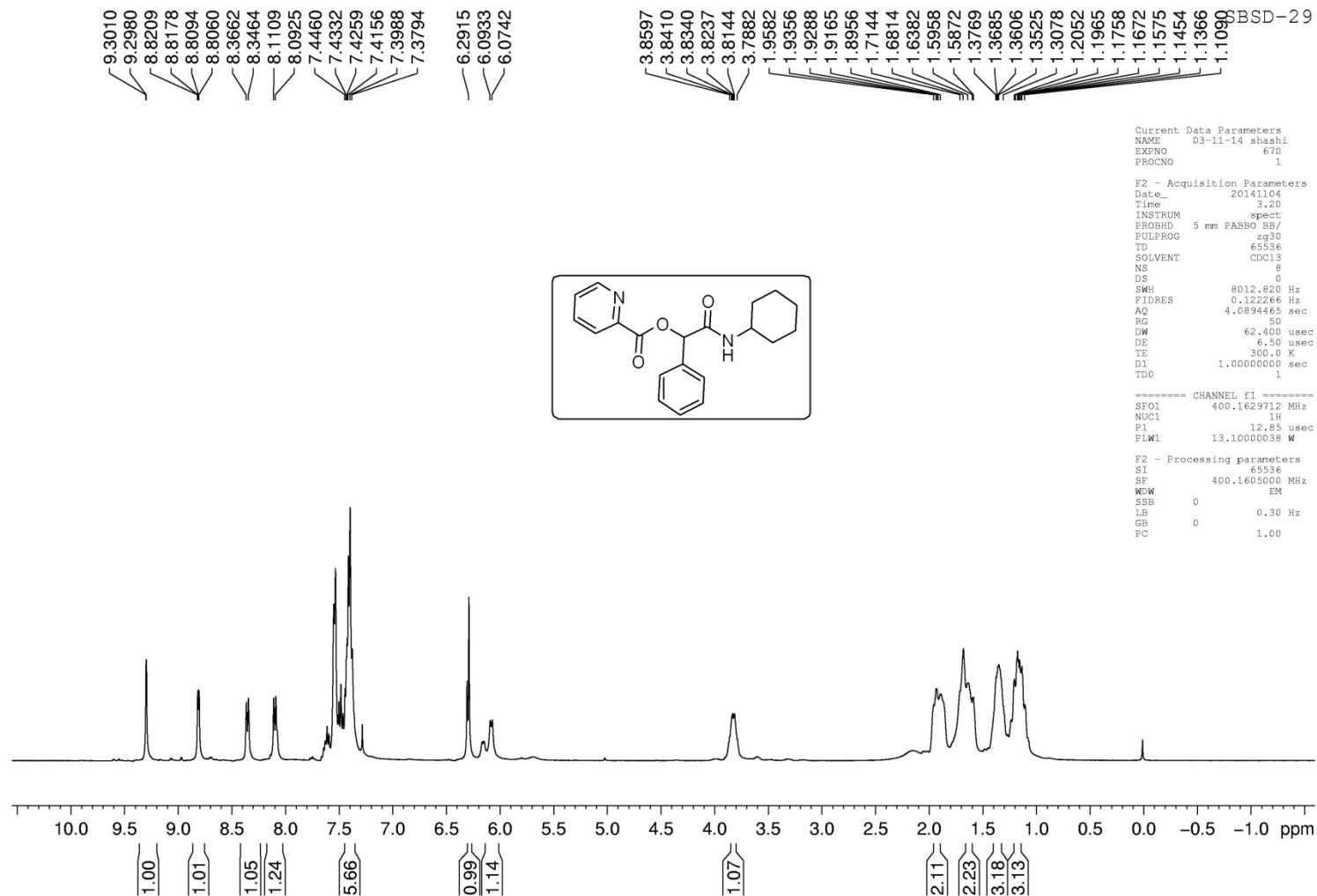


Figure S36. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl nicotinate (4aBa).



**Figure S37.**  $^1\text{H-NMR}$  spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl nicotinate (**4aBb**).

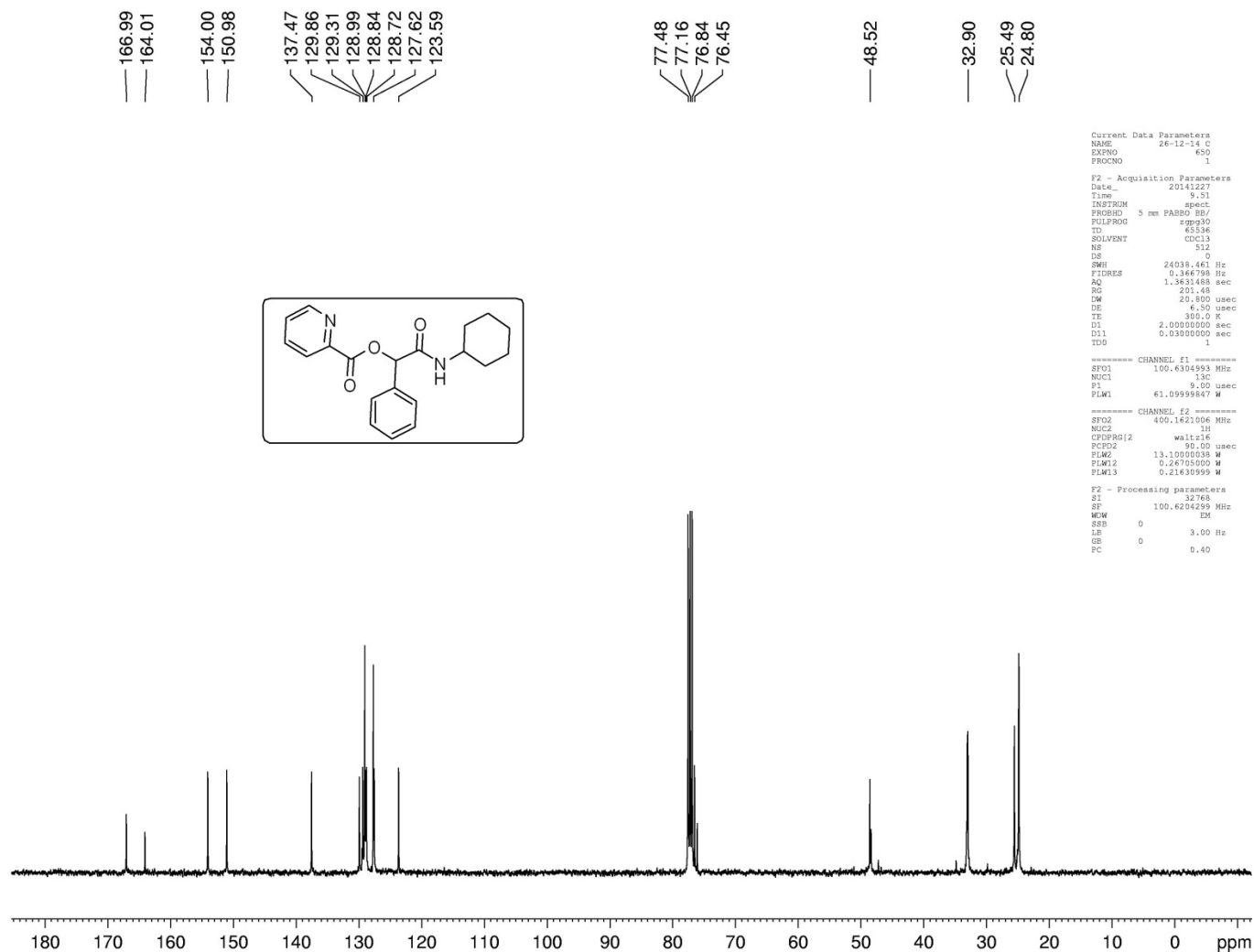


Figure S38.  $^{13}\text{C}$ -NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl nicotinate (**4aBb**).

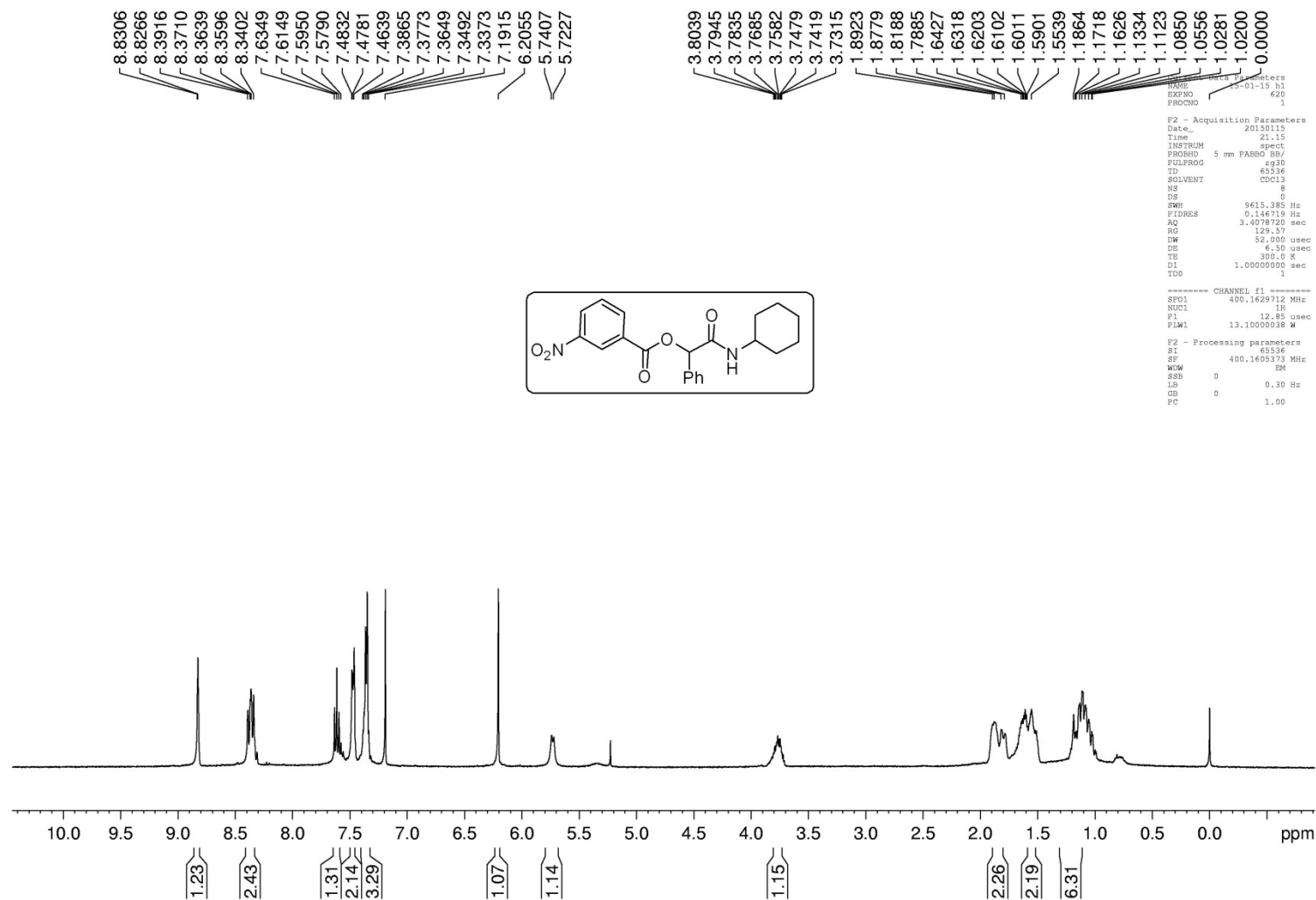
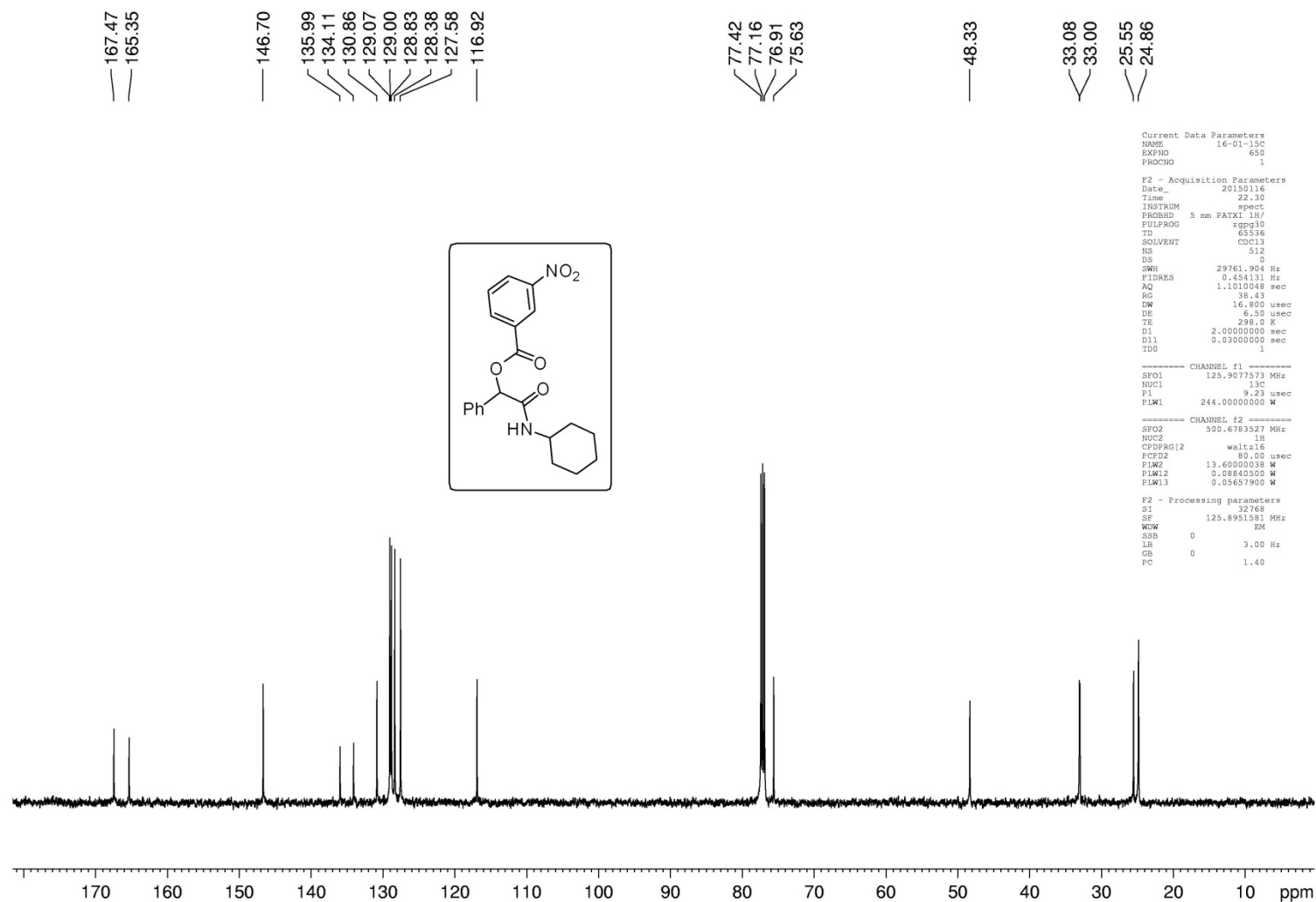
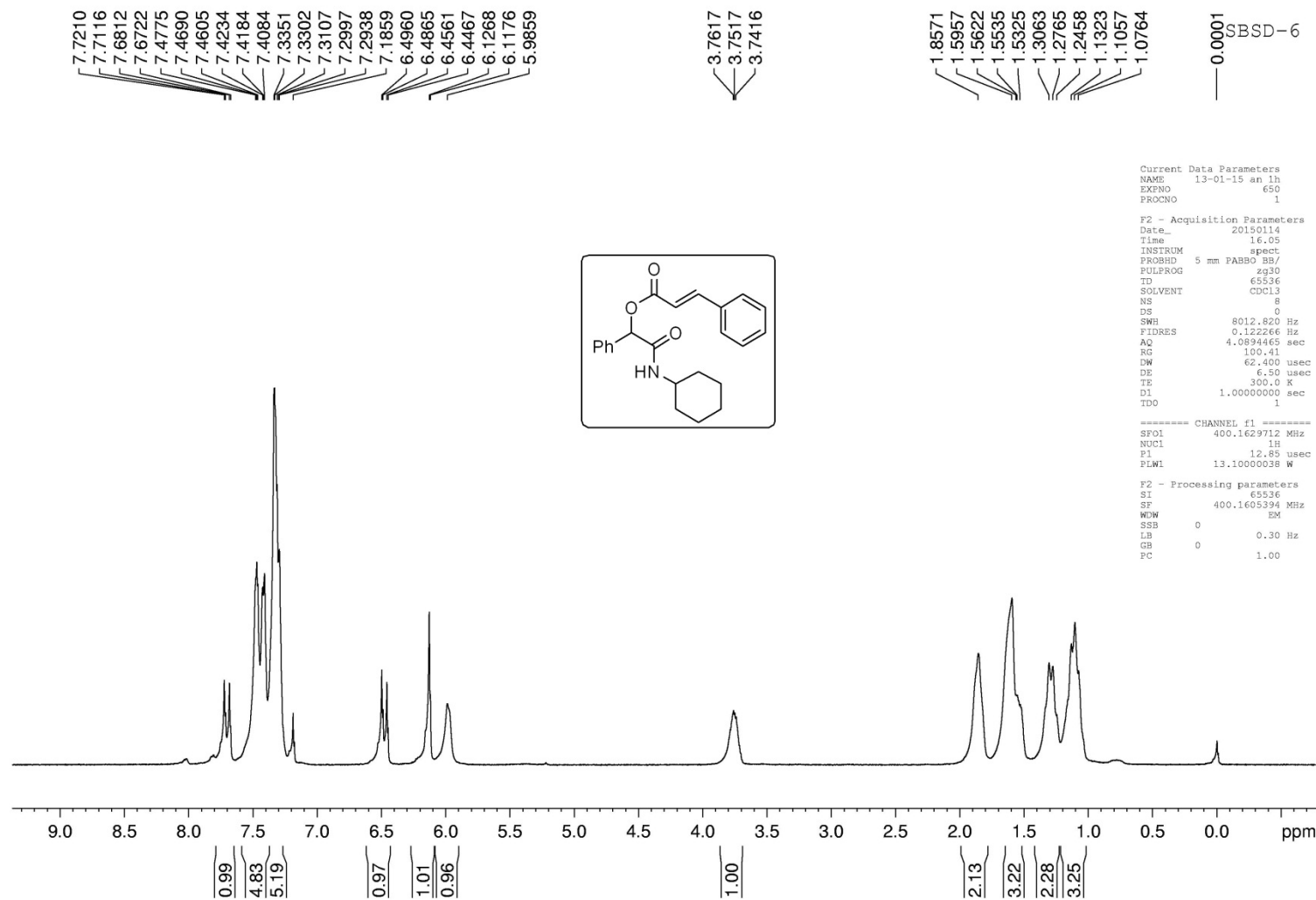


Figure S39. <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl 3-nitrobenzoate (4aCb).





**Figure S40.**  $^{13}\text{C}$ -NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl 3-nitrobenzoate (**4aCb**).



**Figure S41.**  $^1\text{H}$ -NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl cinnamate (**4aDb**).

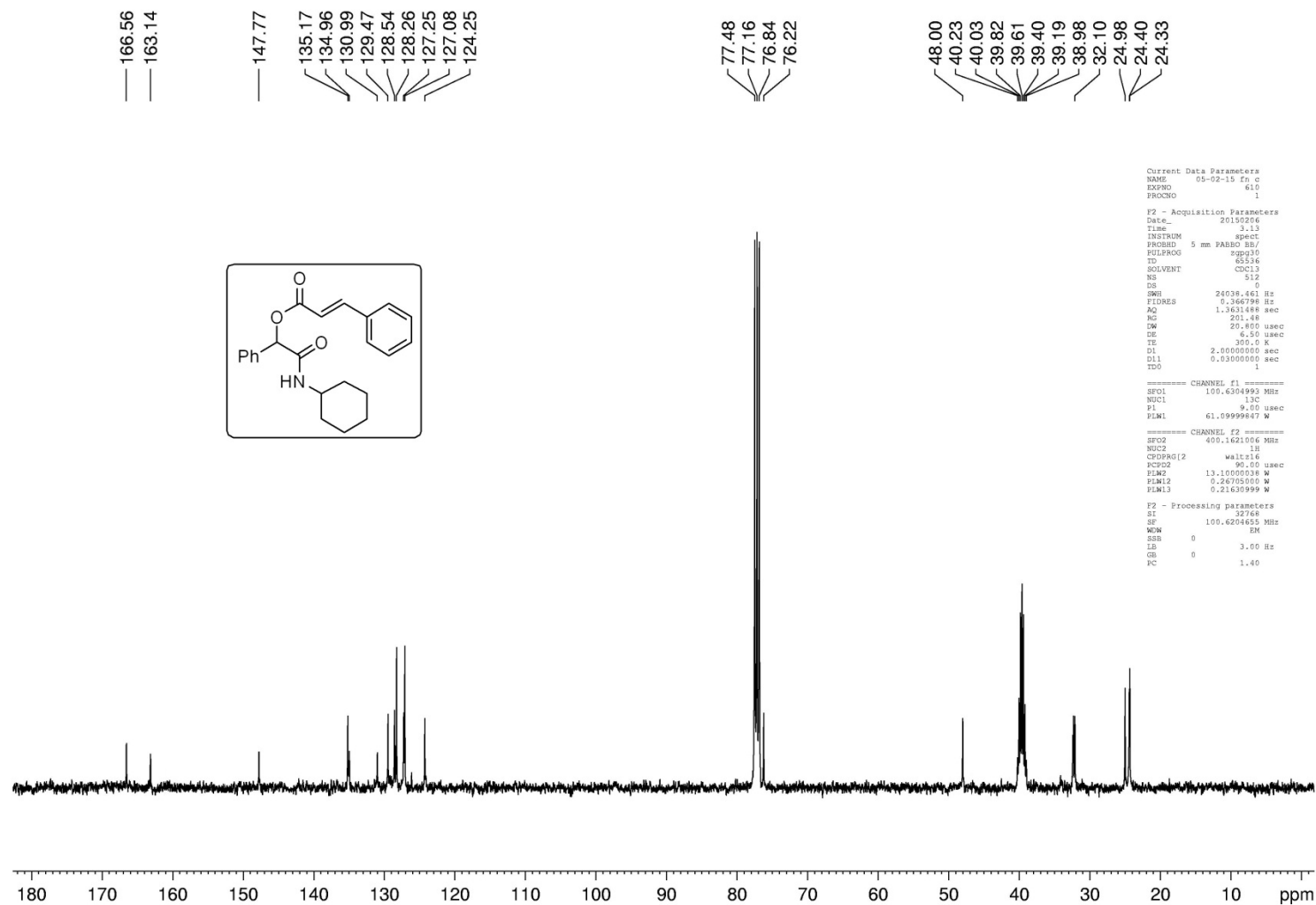
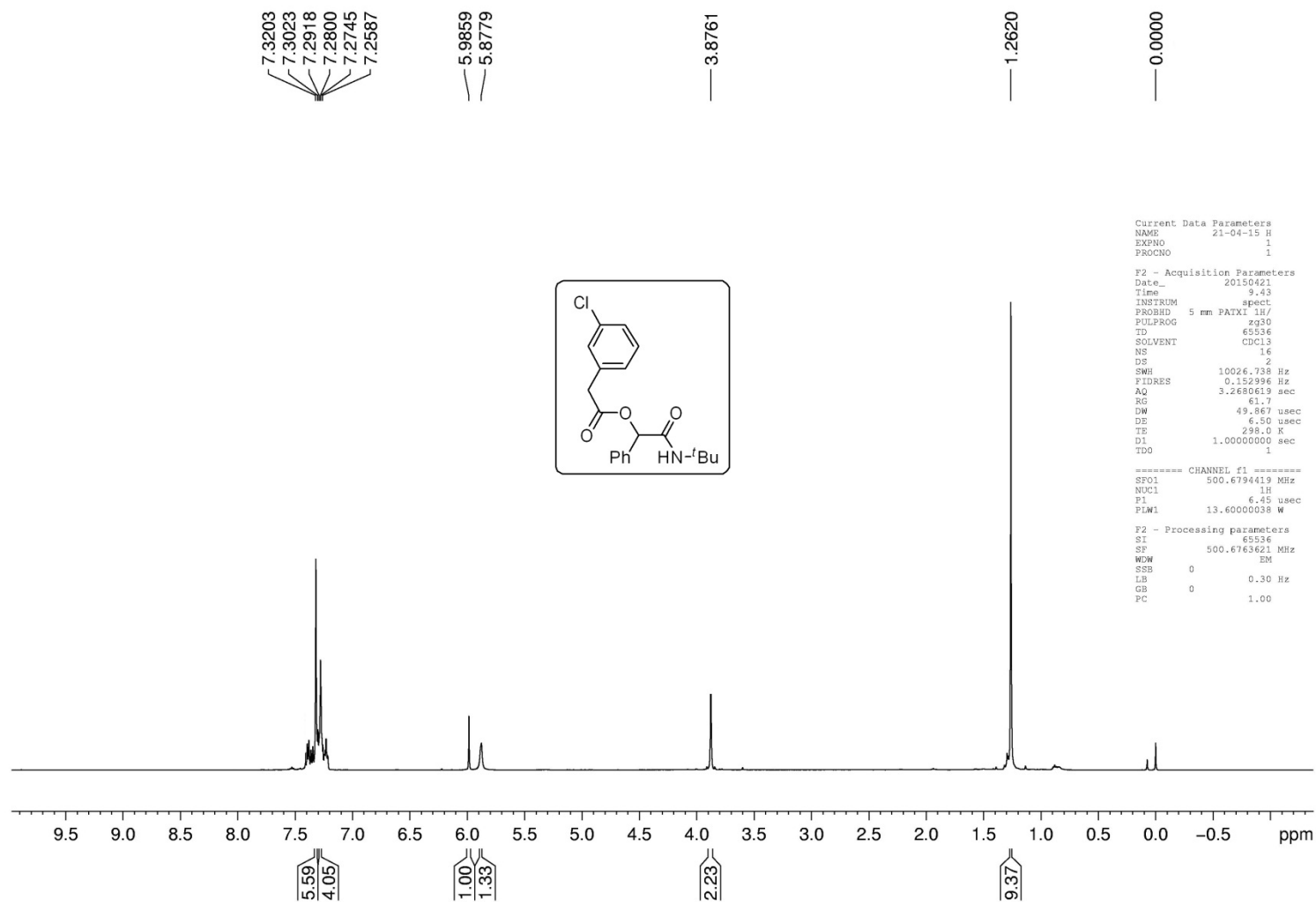
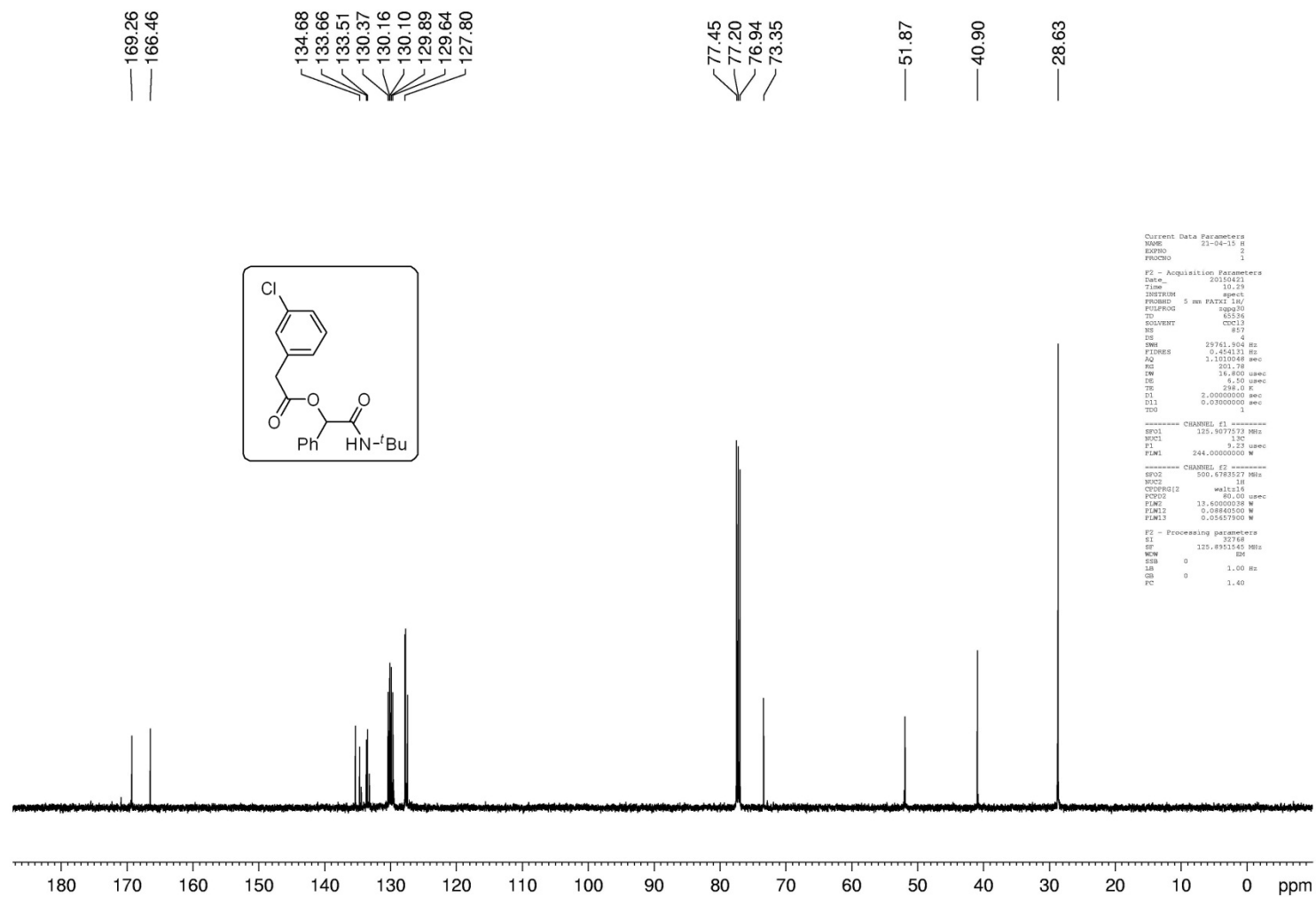


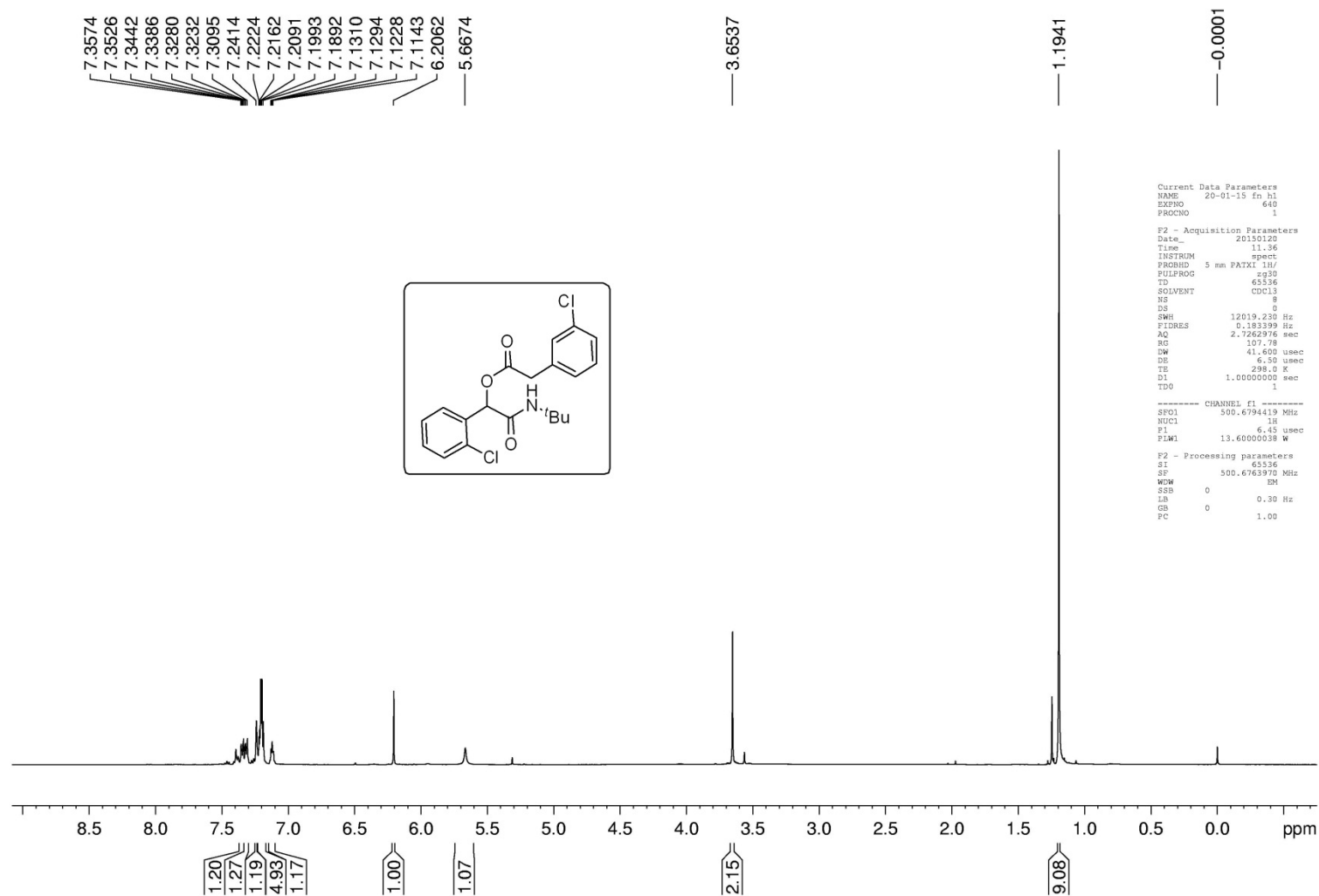
Figure S42.  $^{13}\text{C}$ -NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl cinnamate (4aDb).



**Figure S43.**  $^1\text{H-NMR}$  spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl 2-(3-chlorophenyl)acetate (**4aEa**).



**Figure S44.**  $^{13}\text{C}$ -NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl 2-(3-chlorophenyl)acetate (**4aEa**).



**Figure S45.**  $^1\text{H-NMR}$  spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (**4bEa**).

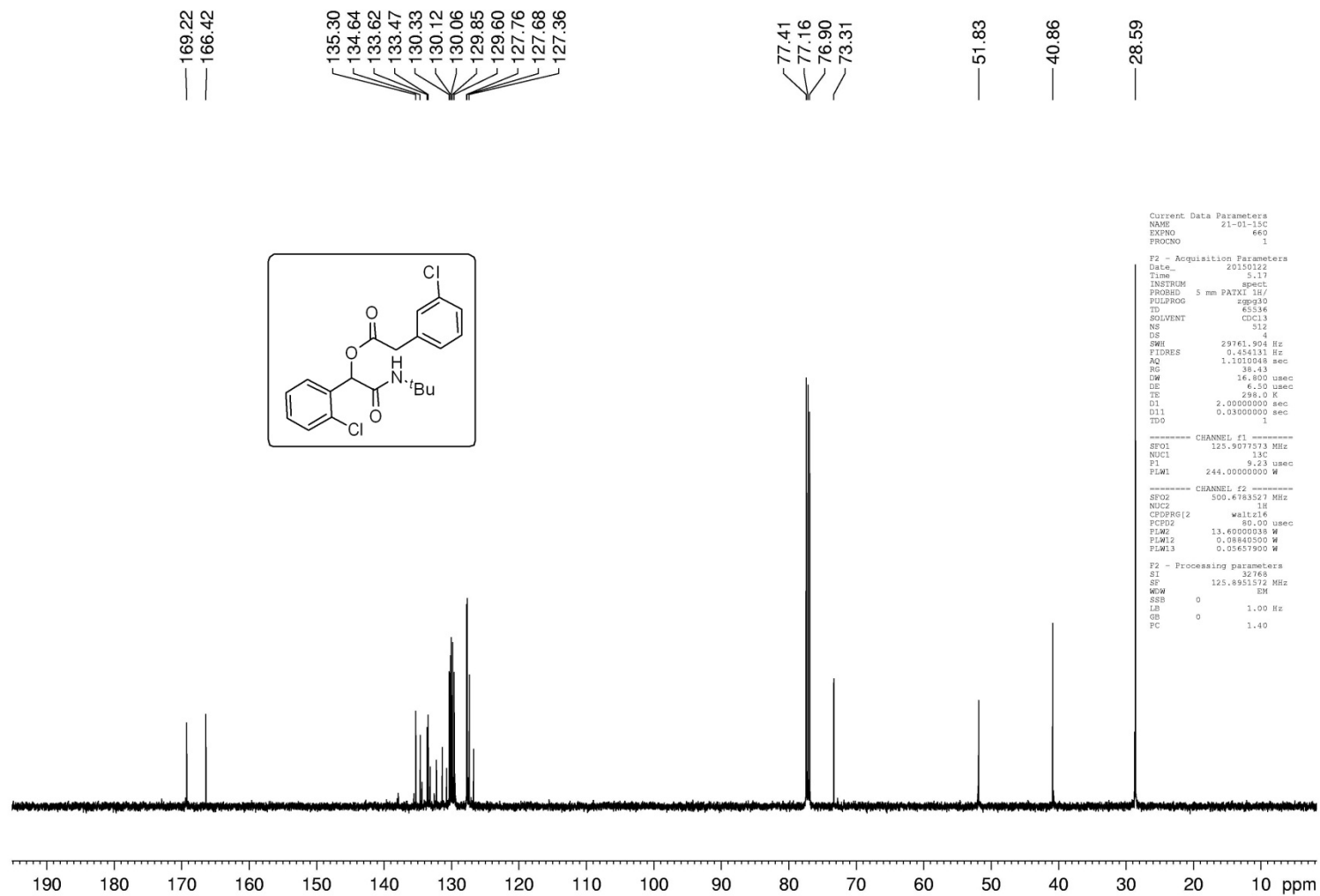
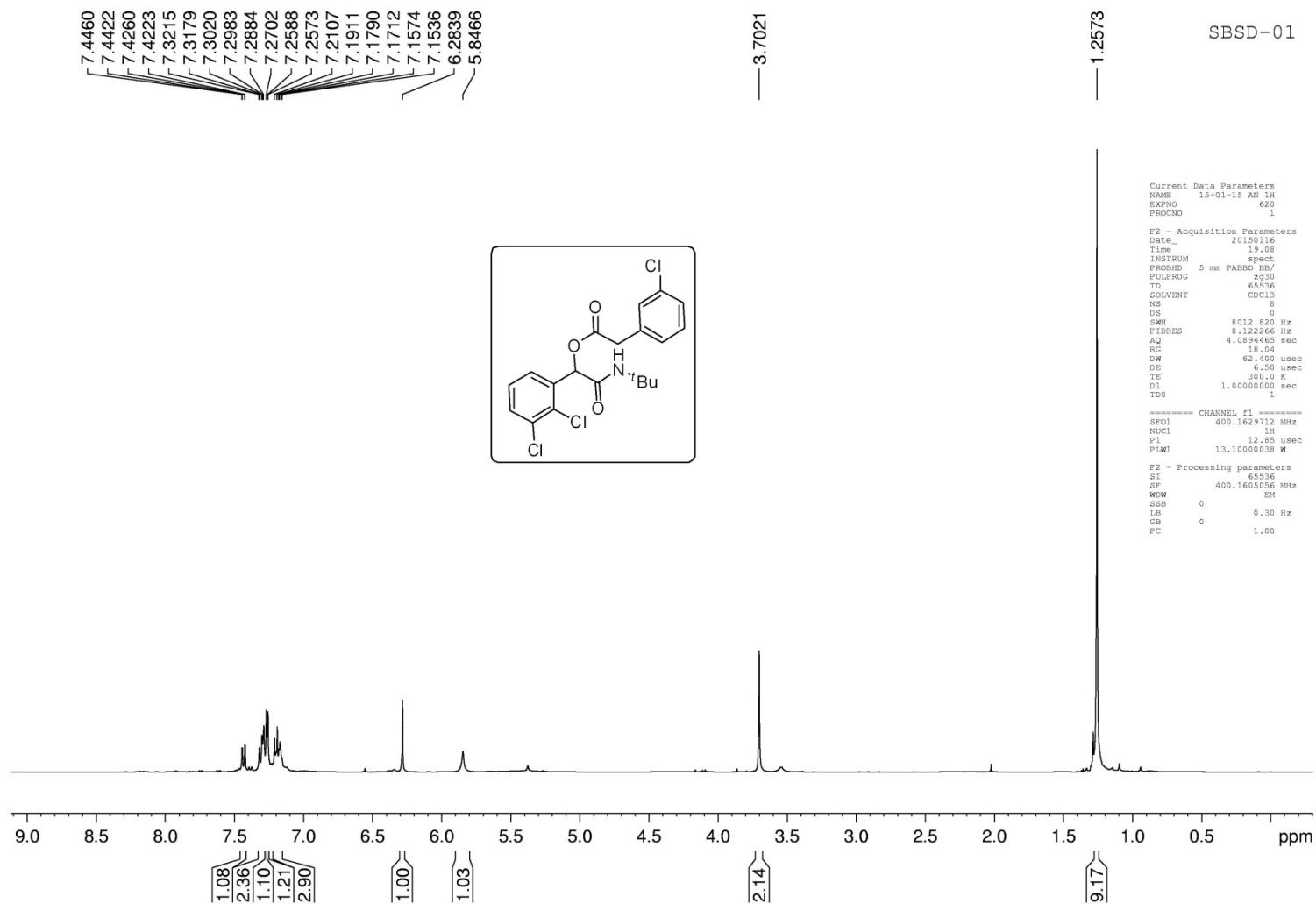


Figure S46.  $^{13}\text{C}$ -NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (**4bEa**).



**Figure S47.**  $^1\text{H-NMR}$  spectrum of 2-(*tert*-butylamino)-1-(2,3-dichlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (**4iEa**).



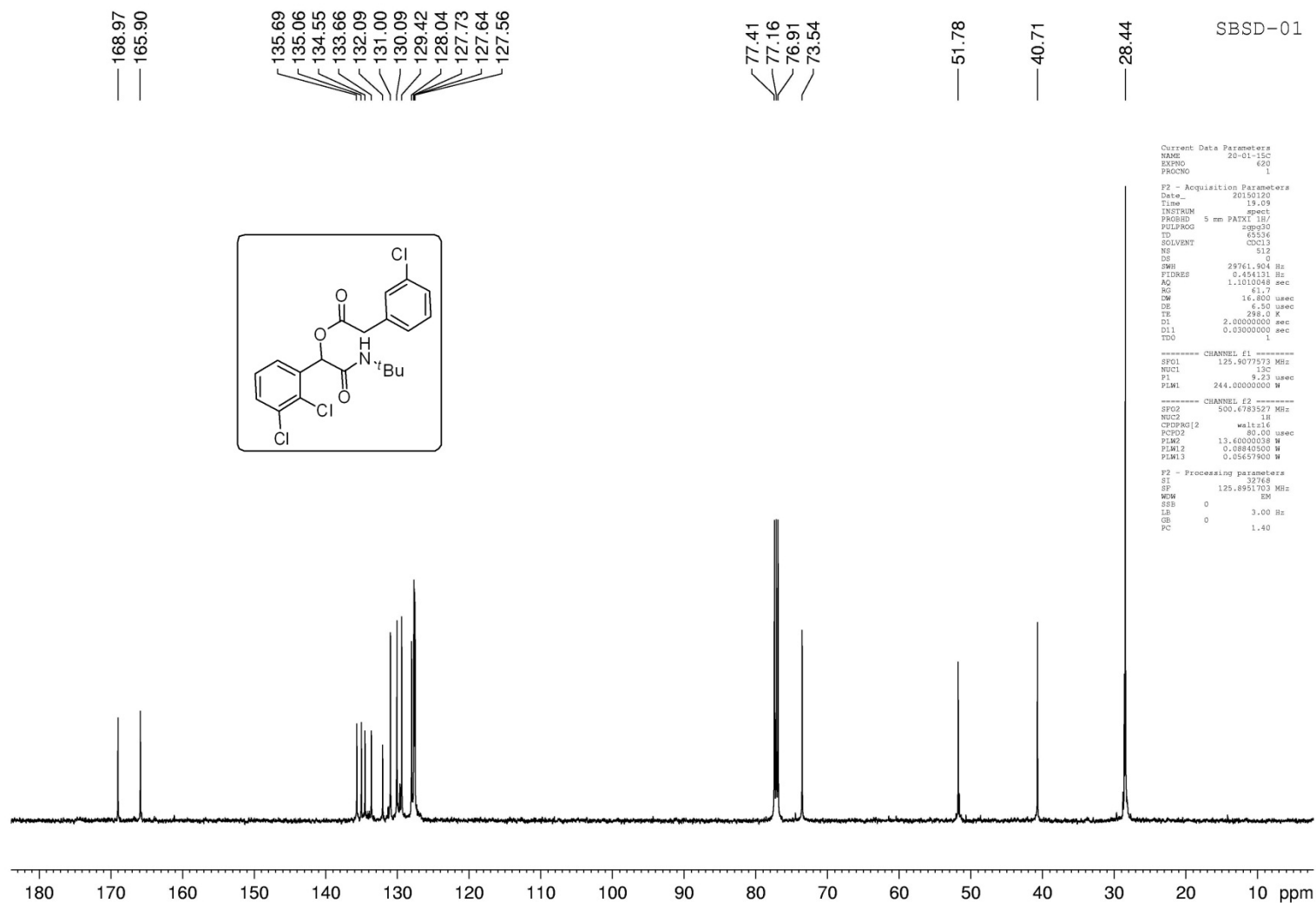


Figure S48.  $^{13}\text{C}$ -NMR spectrum of 2-(*tert*-butylamino)-1-(2,3-dichlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (**4iEa**).