

## Supporting Information

### Mimics of Pramanicin derived from Pyroglutamic acid and their Antibacterial Activity

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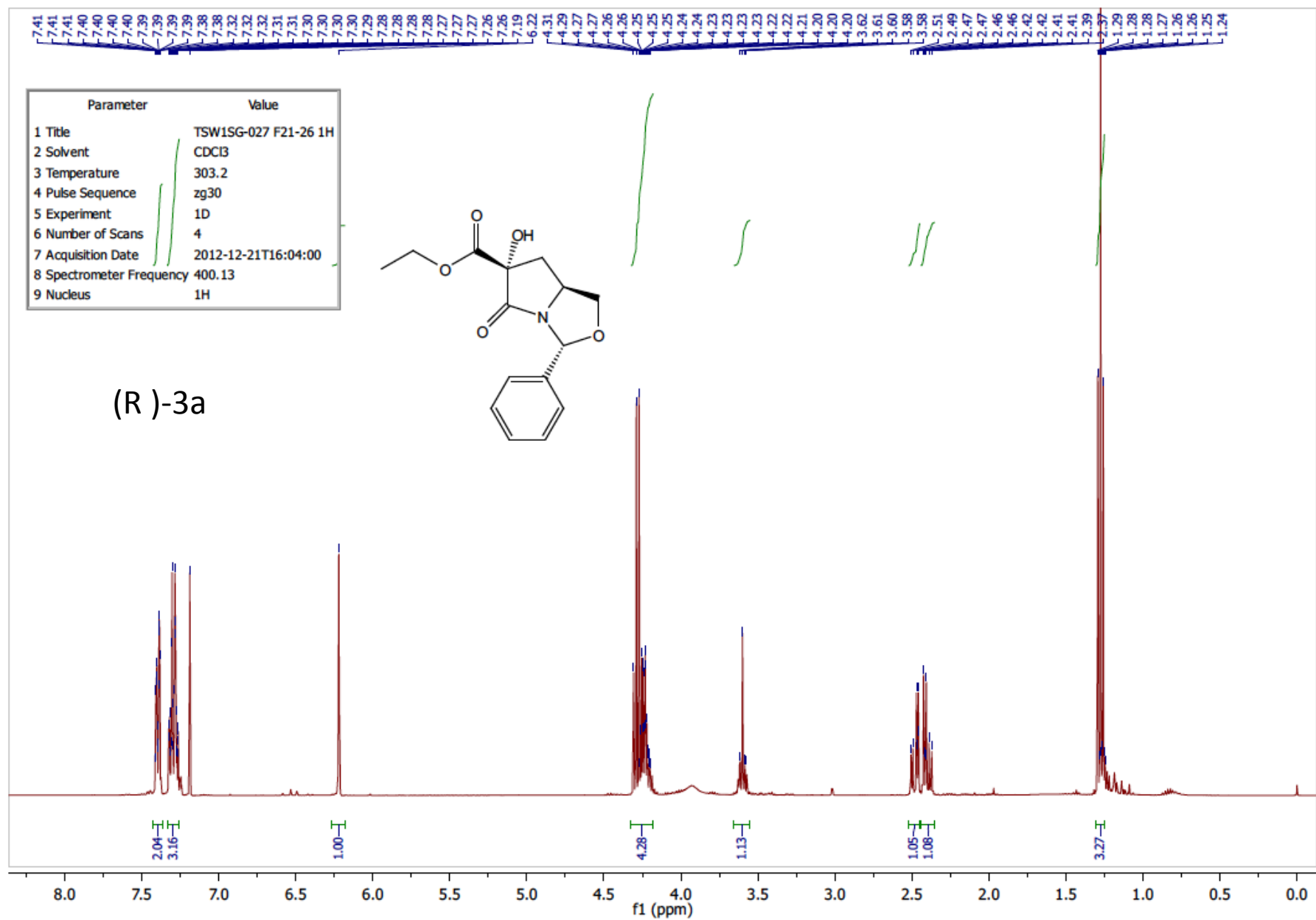
<sup>b</sup>Institute of Chemical and Engineering Sciences (ICES), 8 Biomedical Grove, Neuros Building, #07-01/02/03, Singapore 138665;

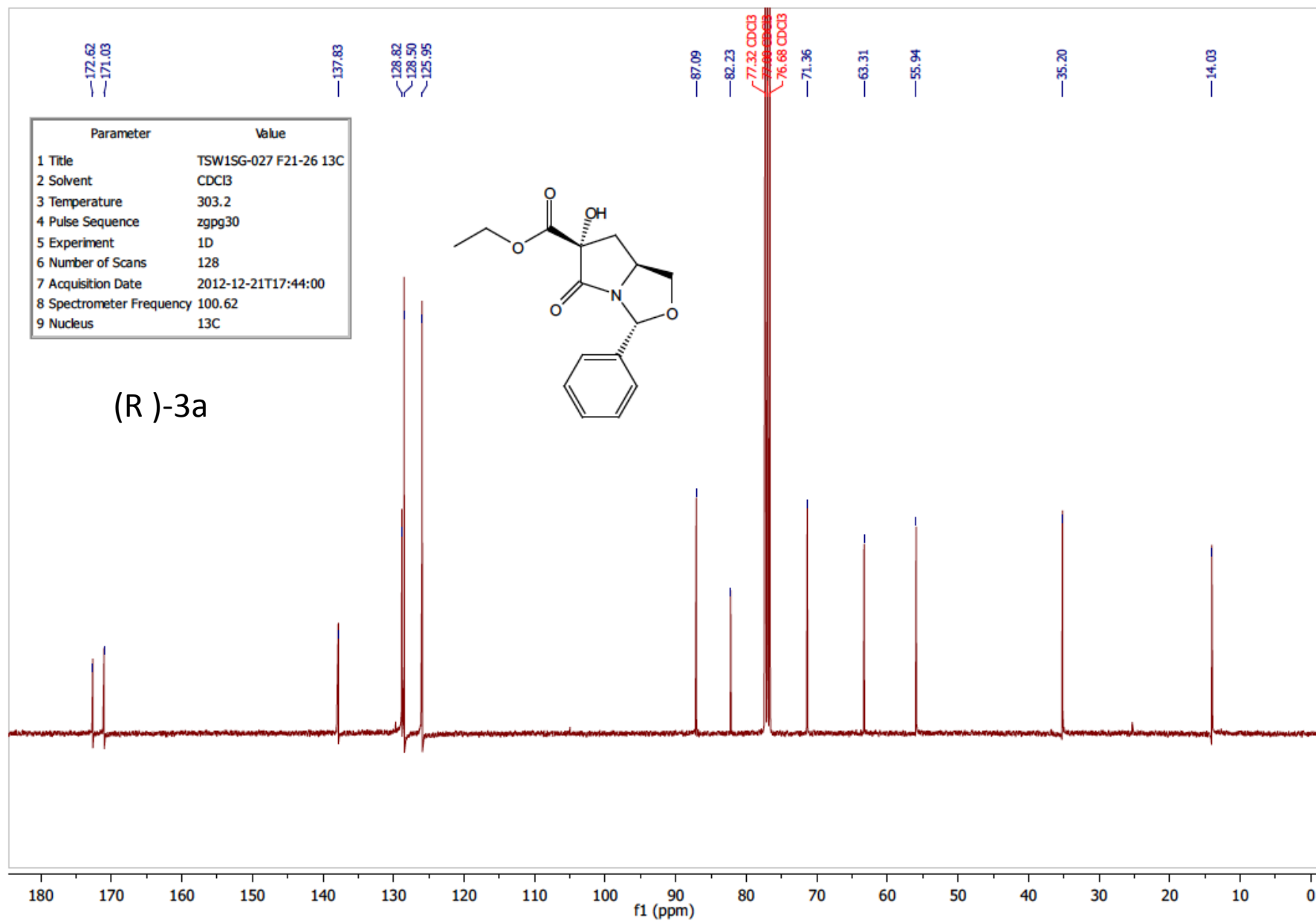
<sup>c</sup>Department of Pharmacy, National University of Singapore, 18 Science Drive 4, Singapore, 117543

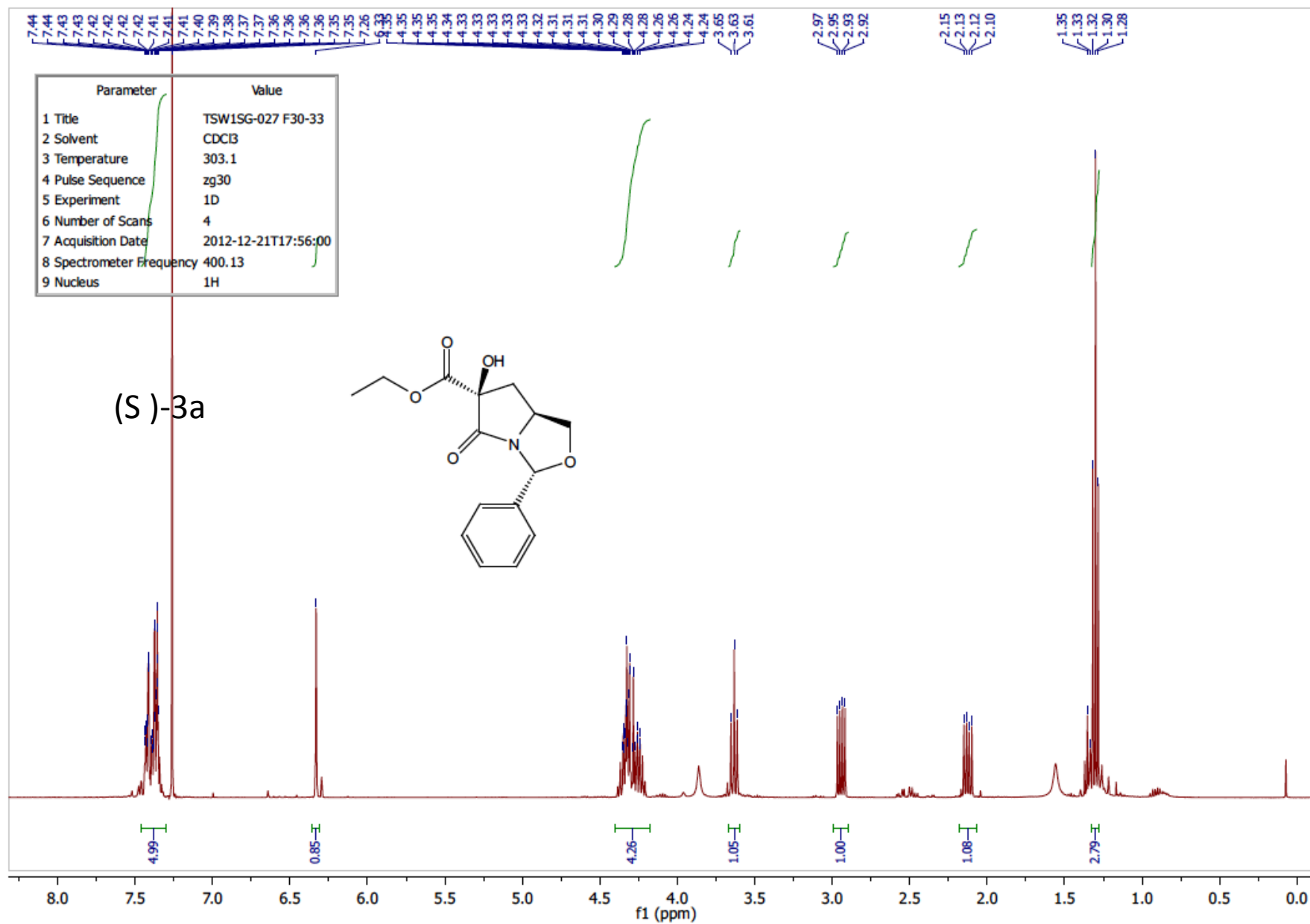
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christina\_chai@ices.a-star.edu.sg

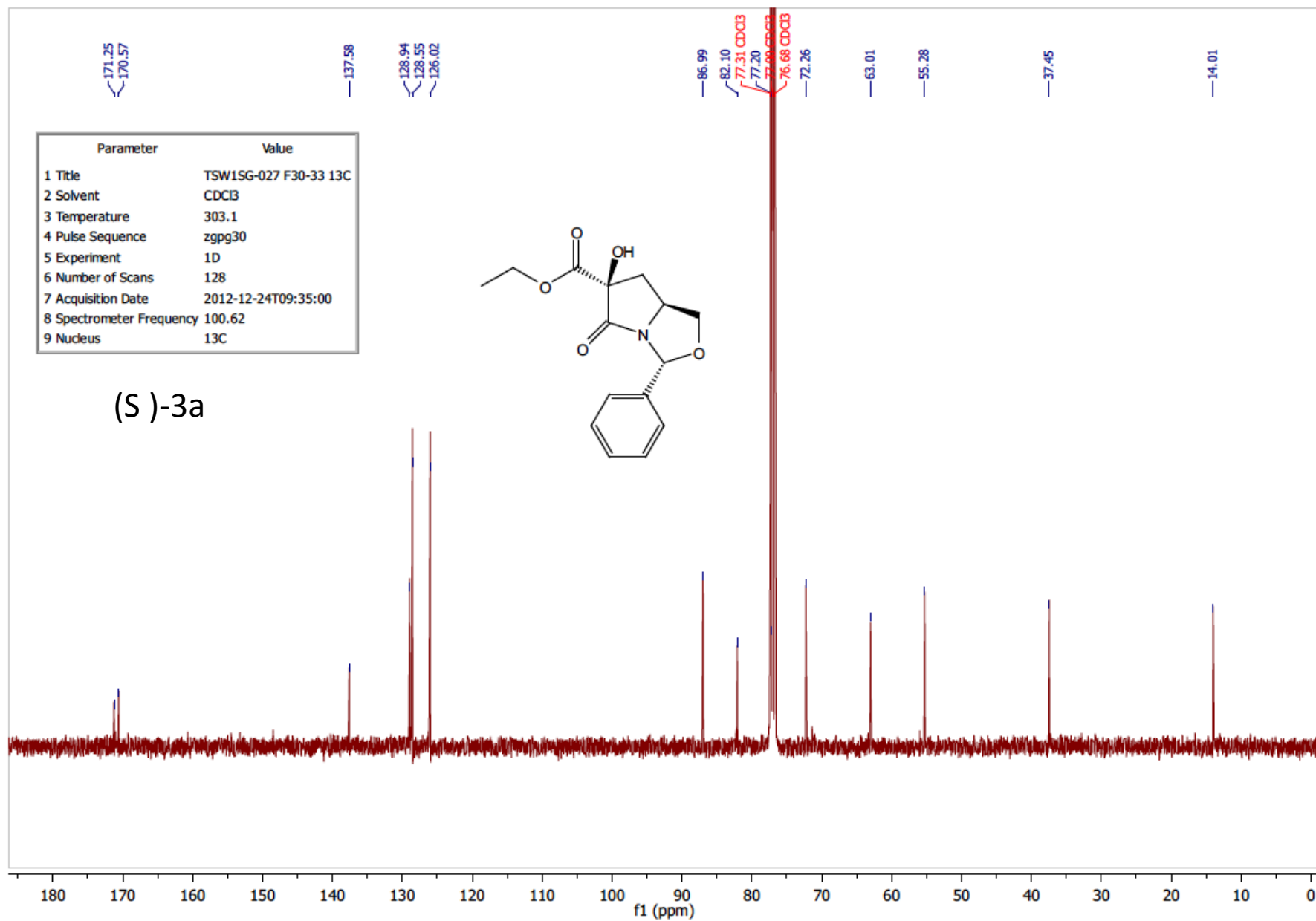
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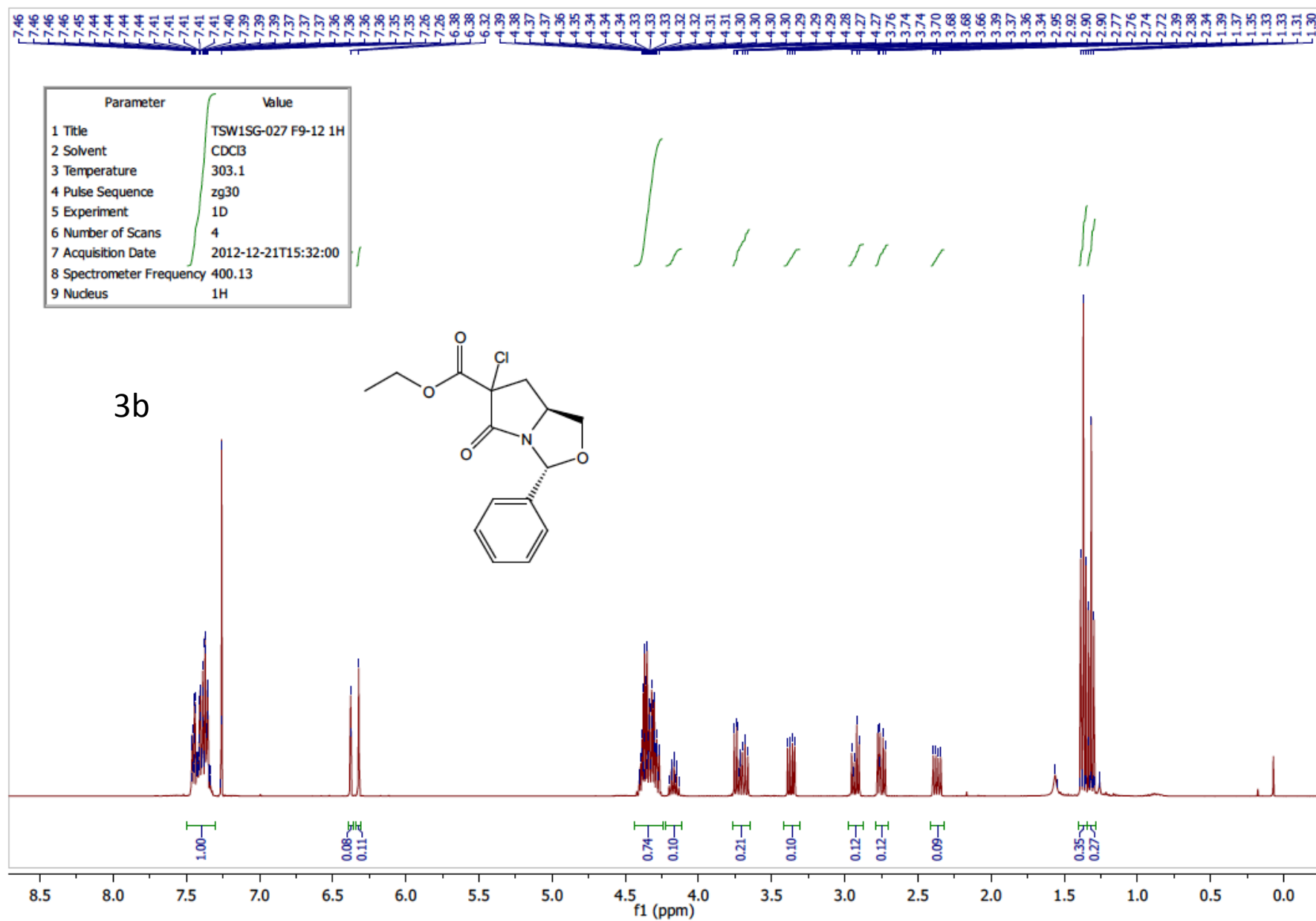
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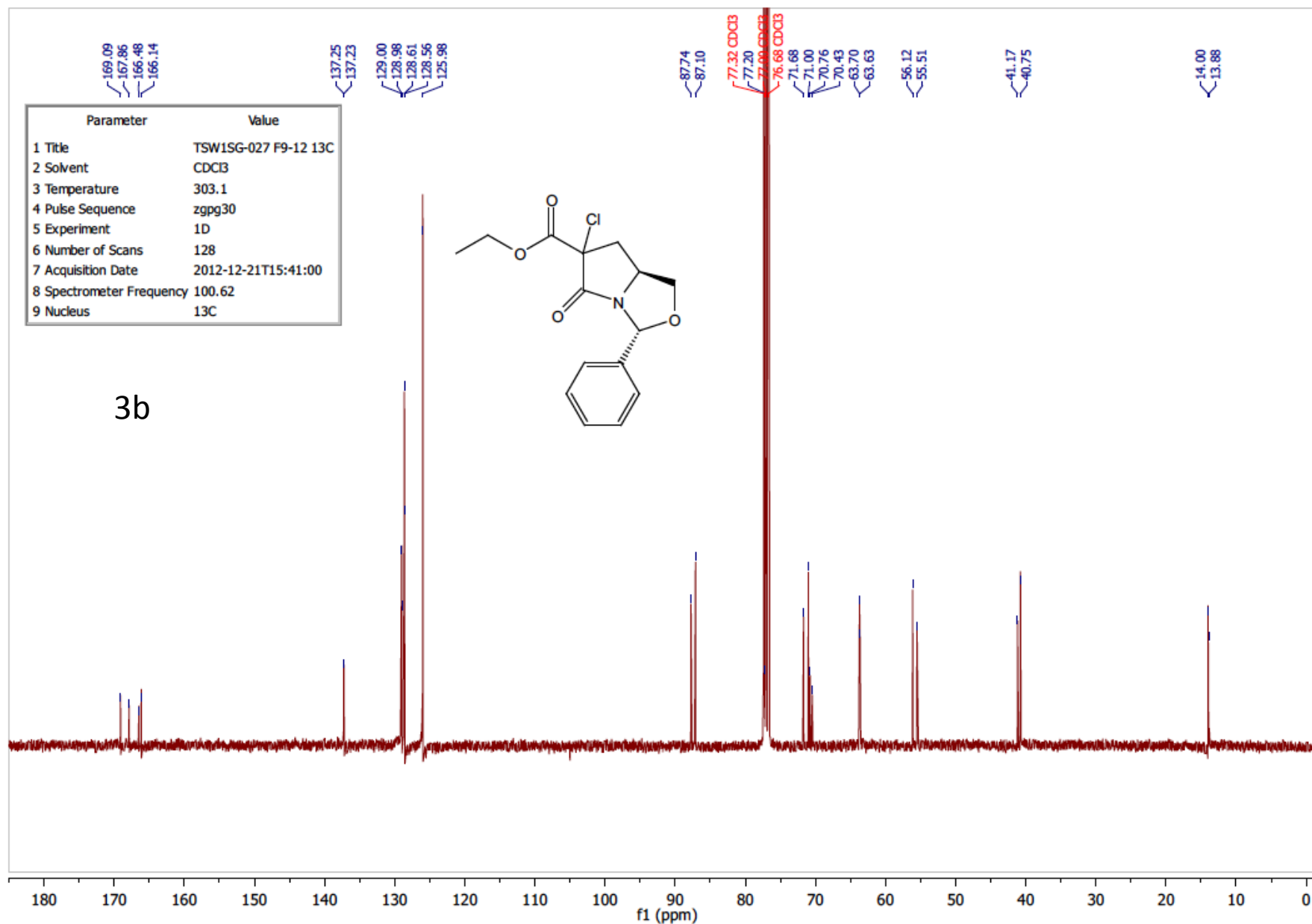


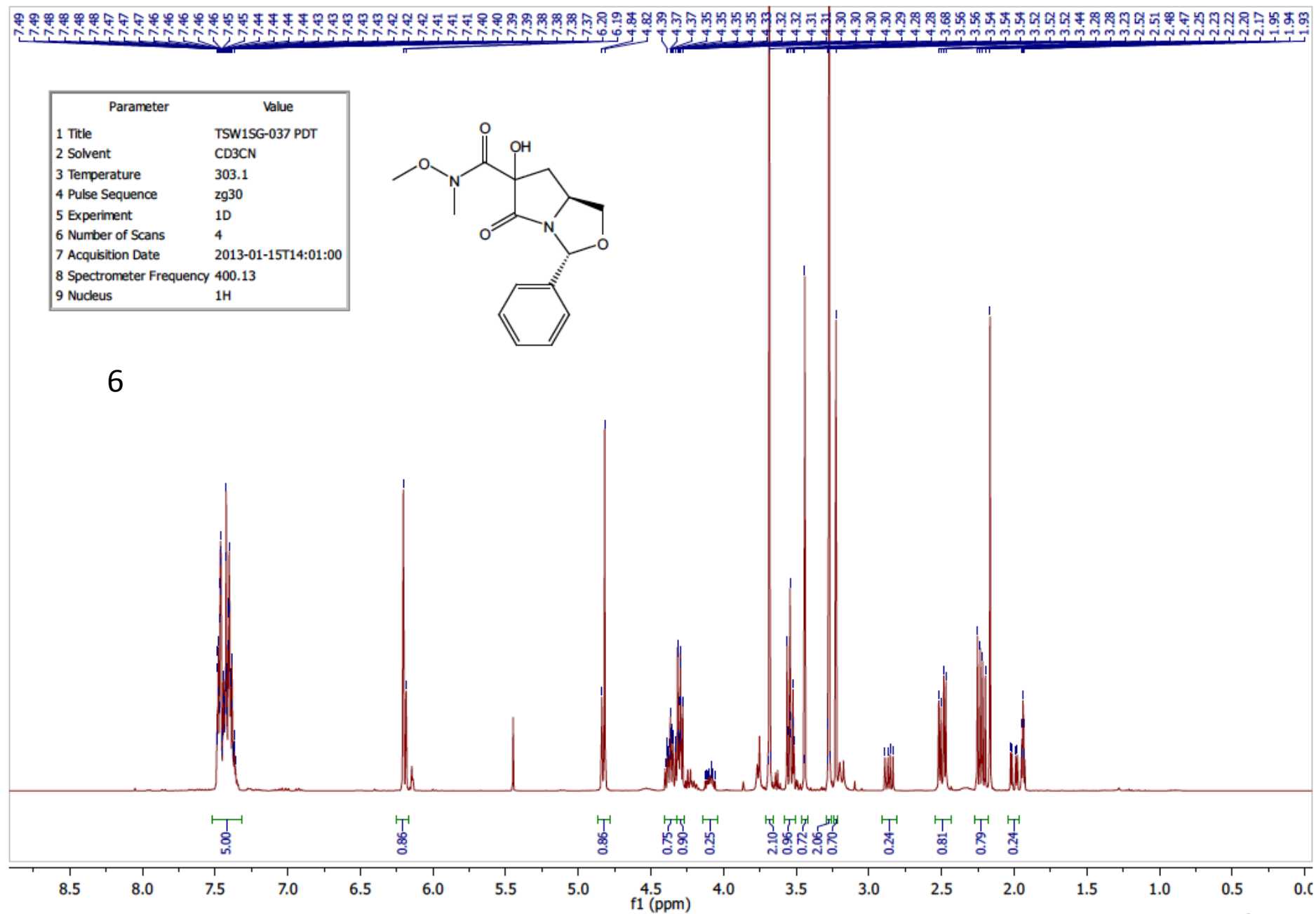


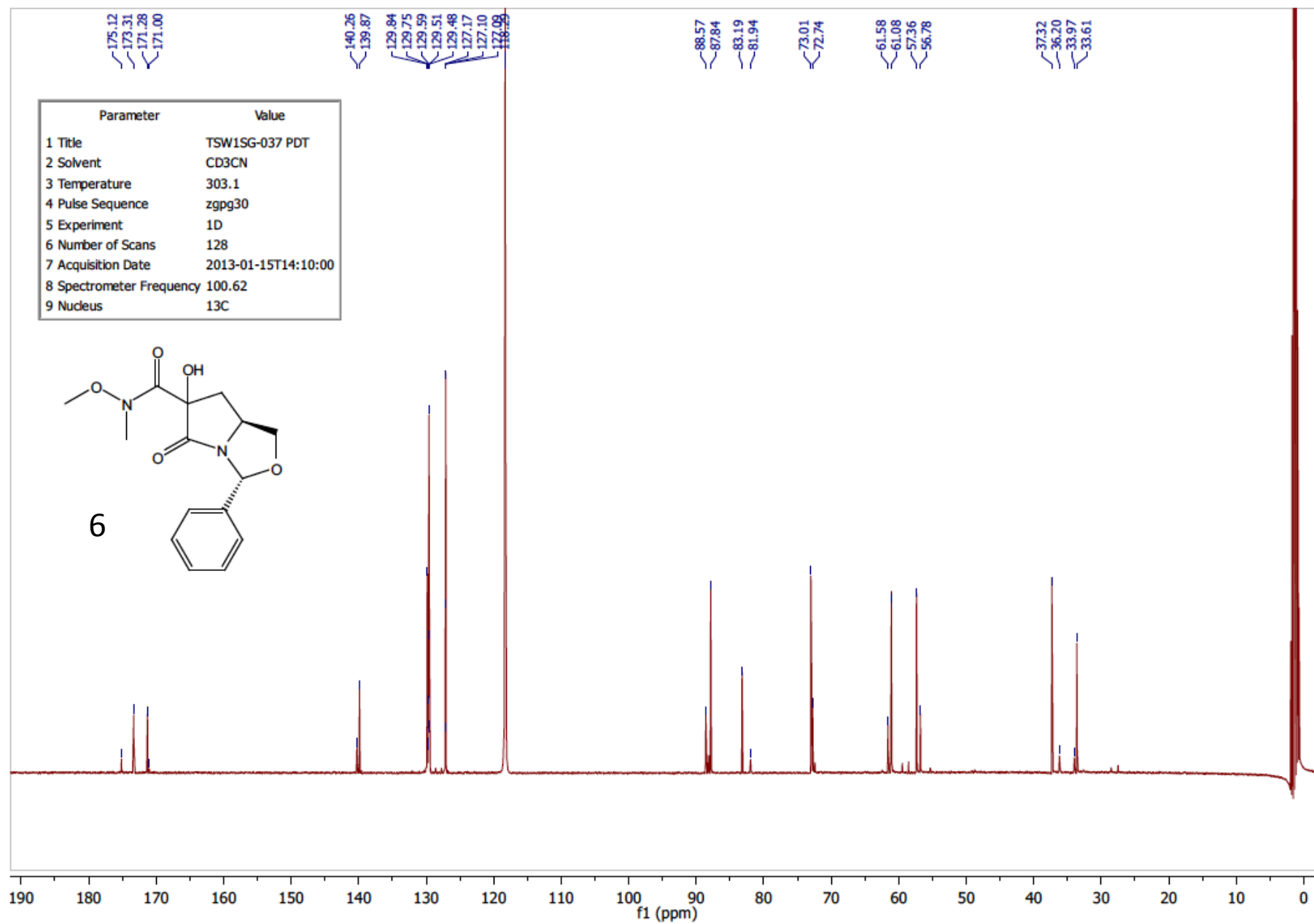


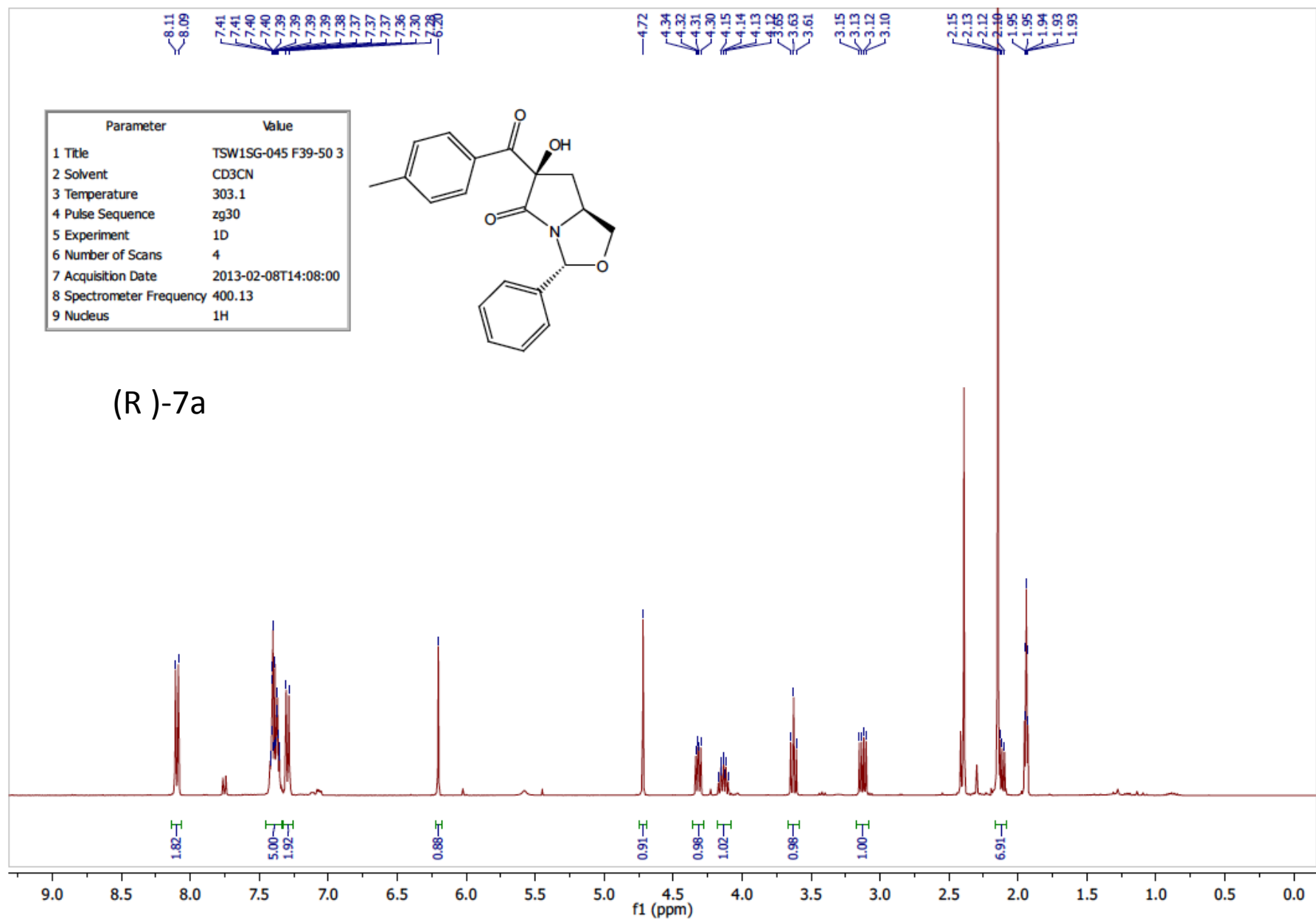


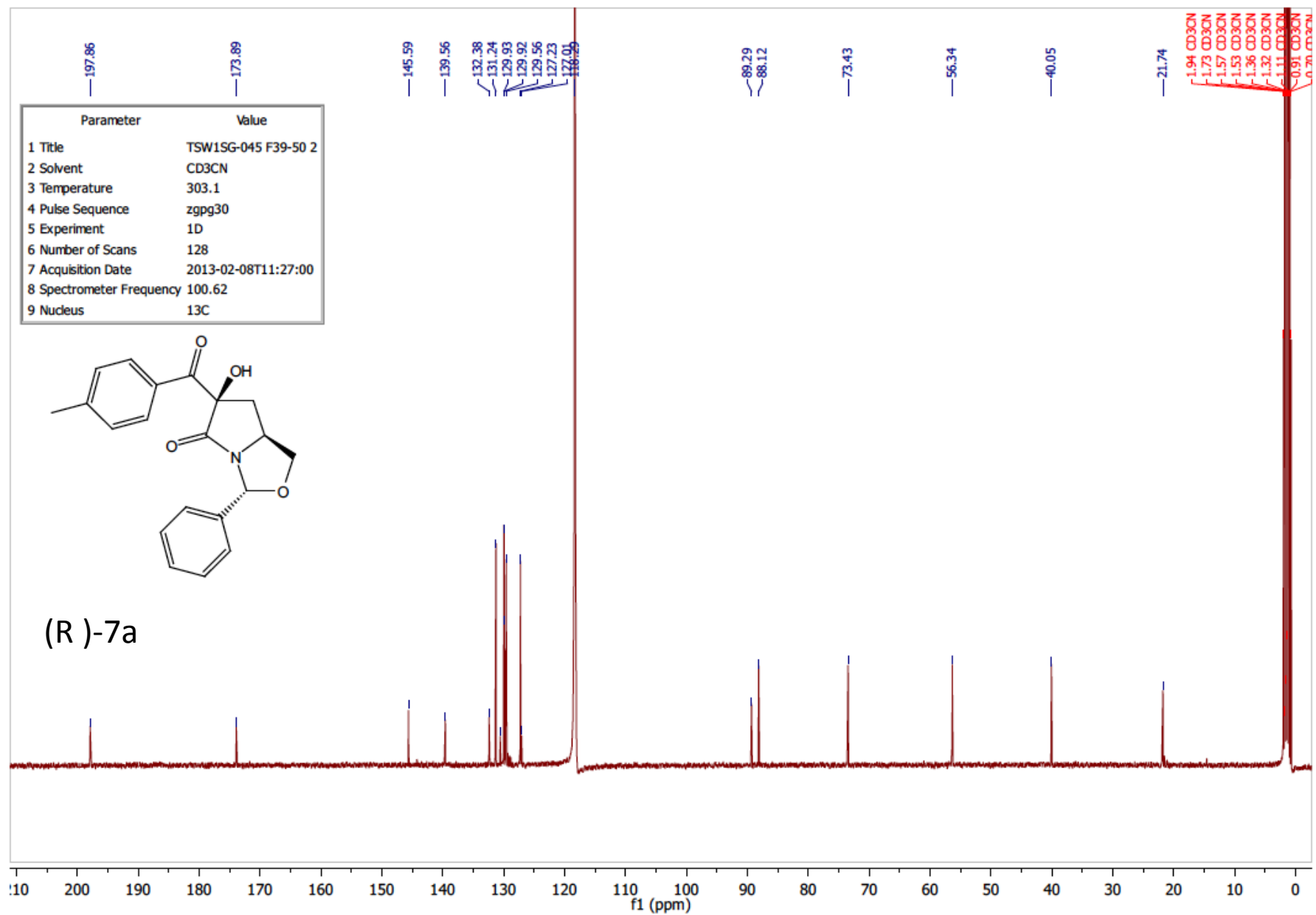




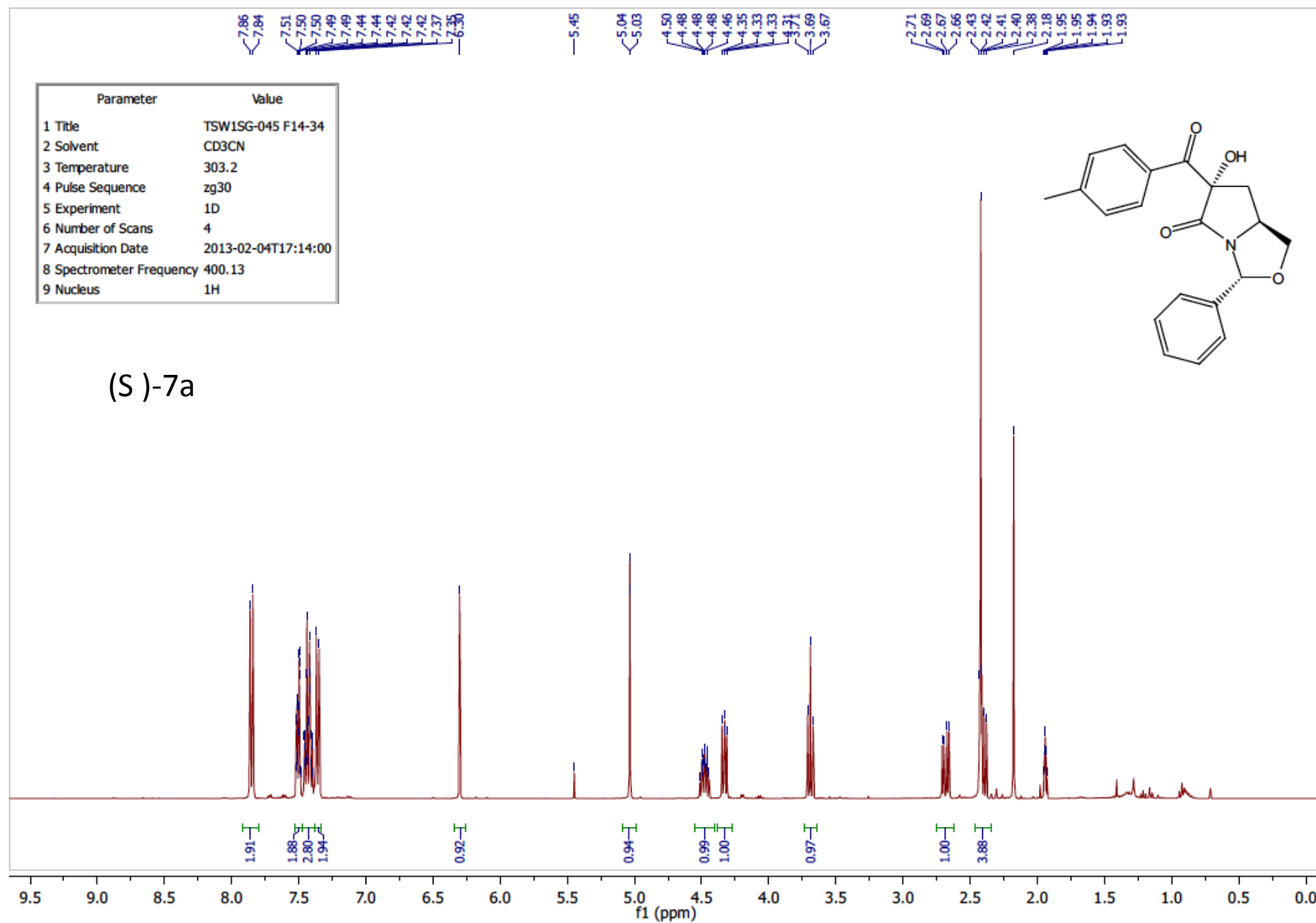


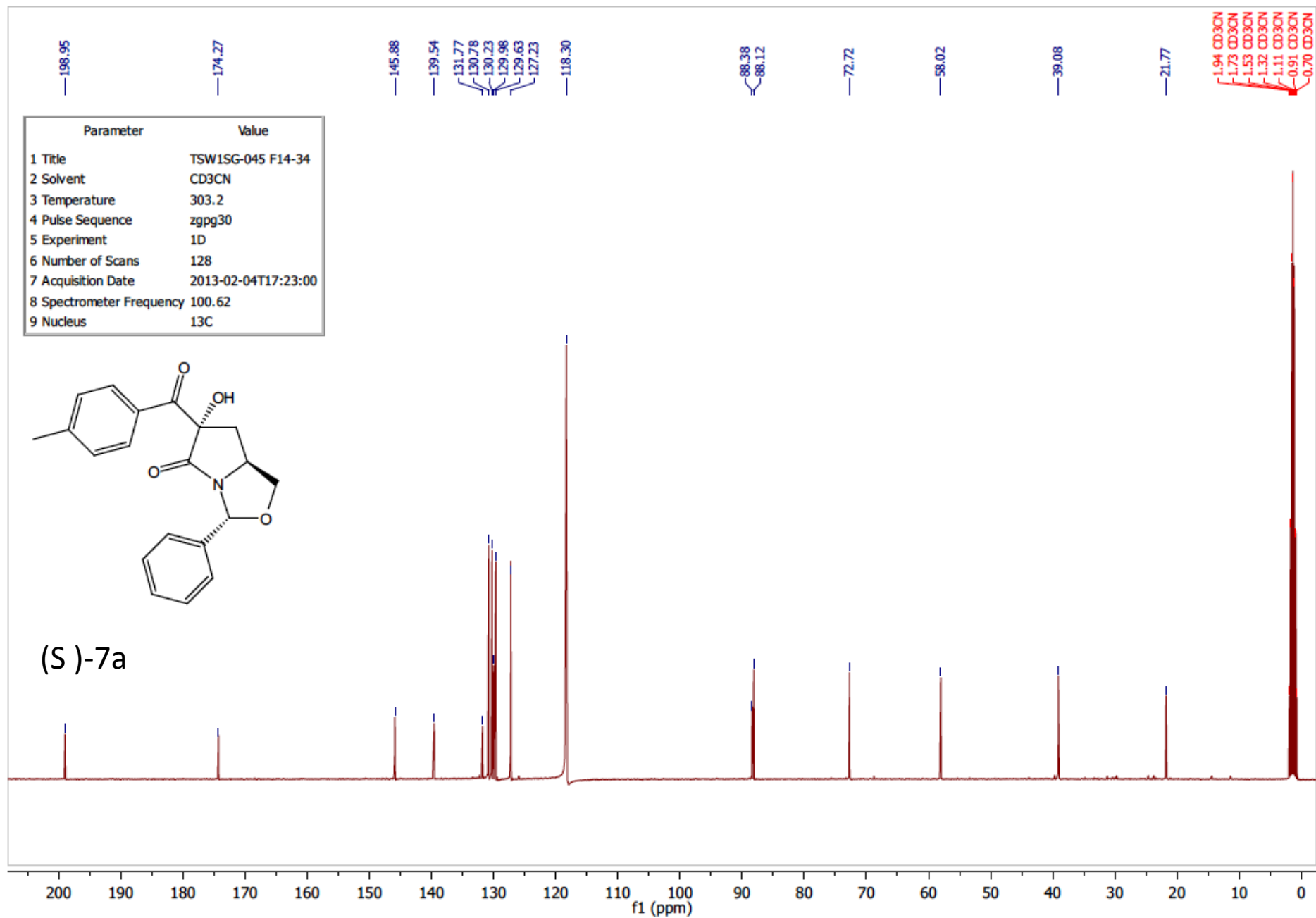


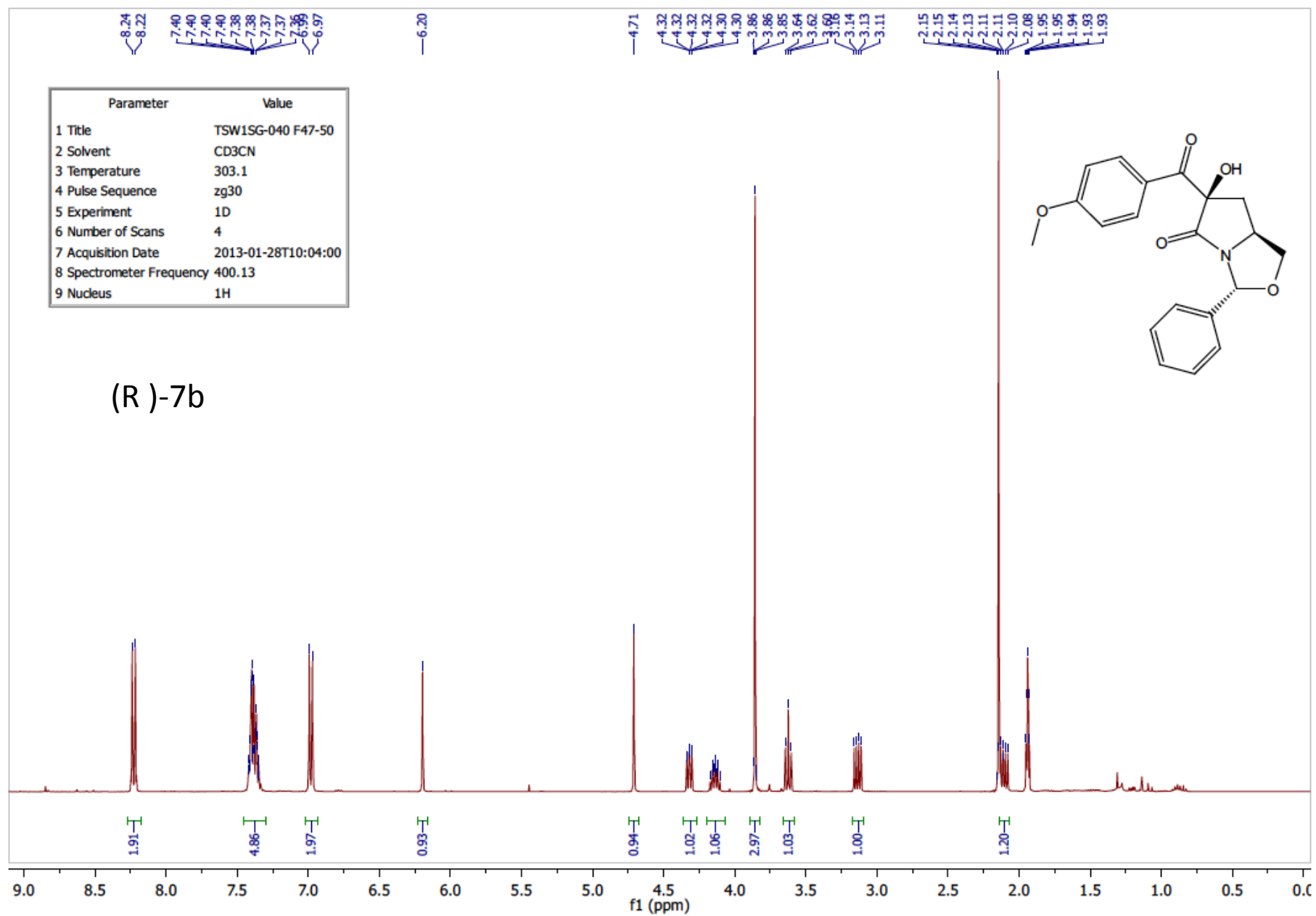


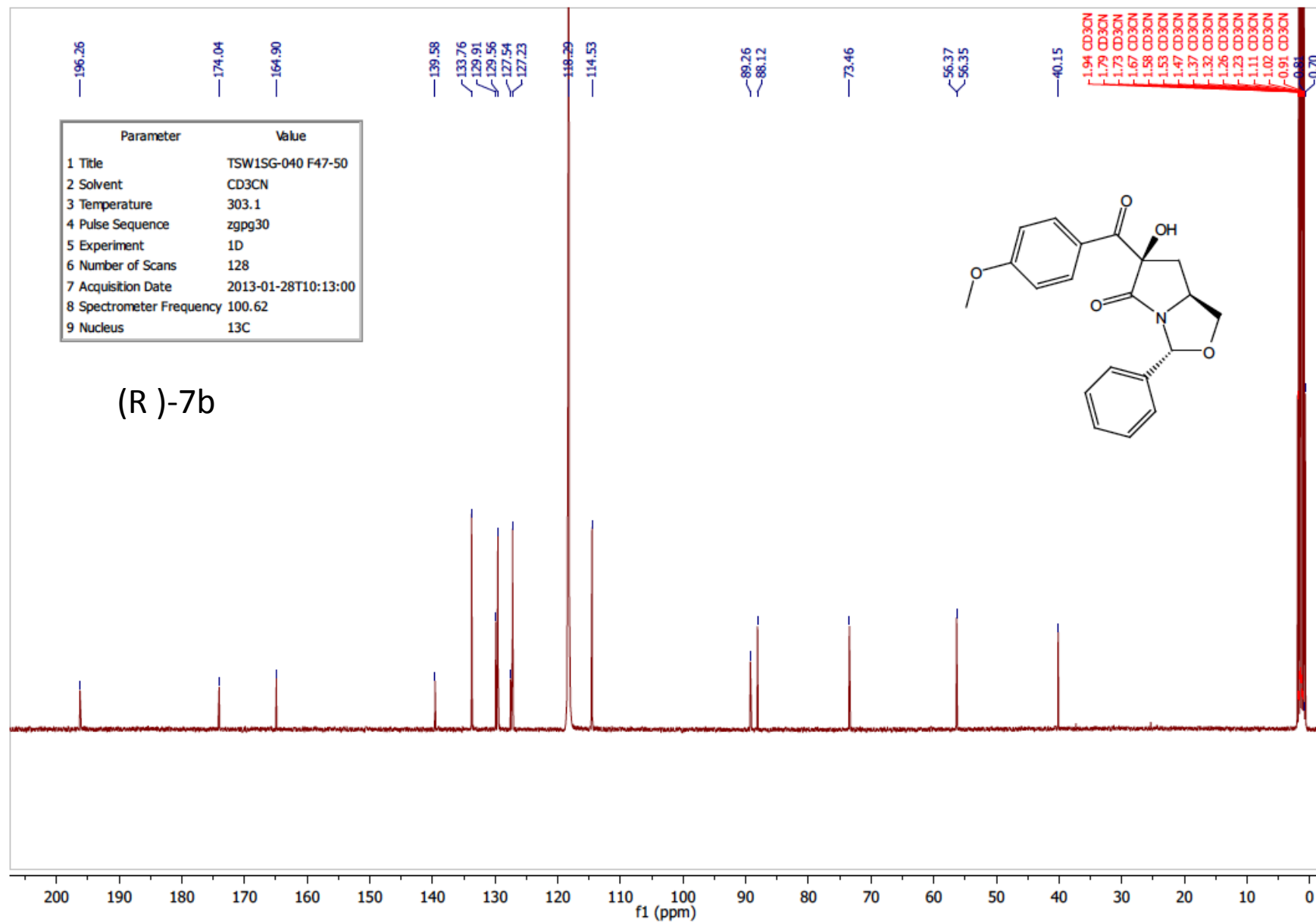


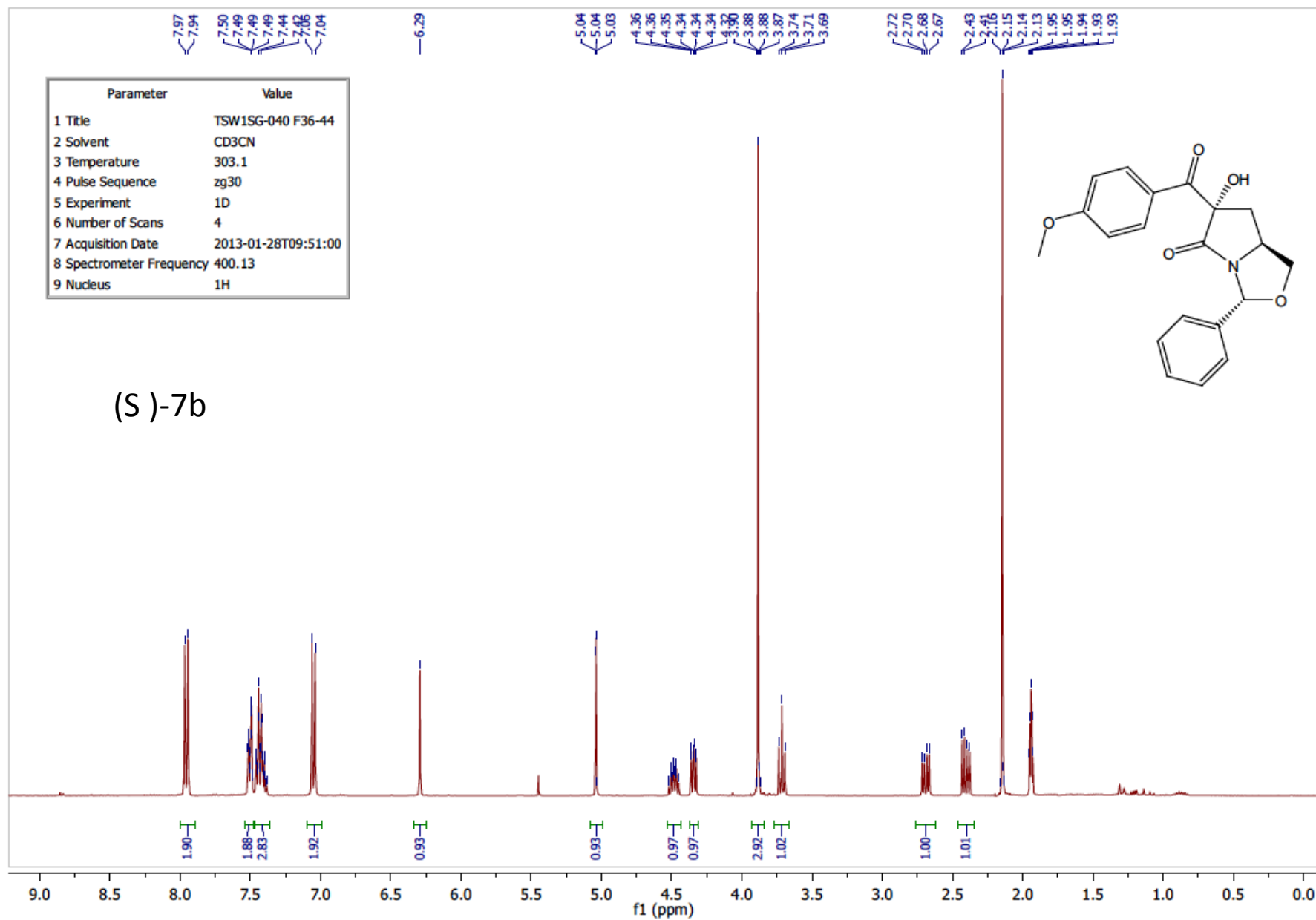
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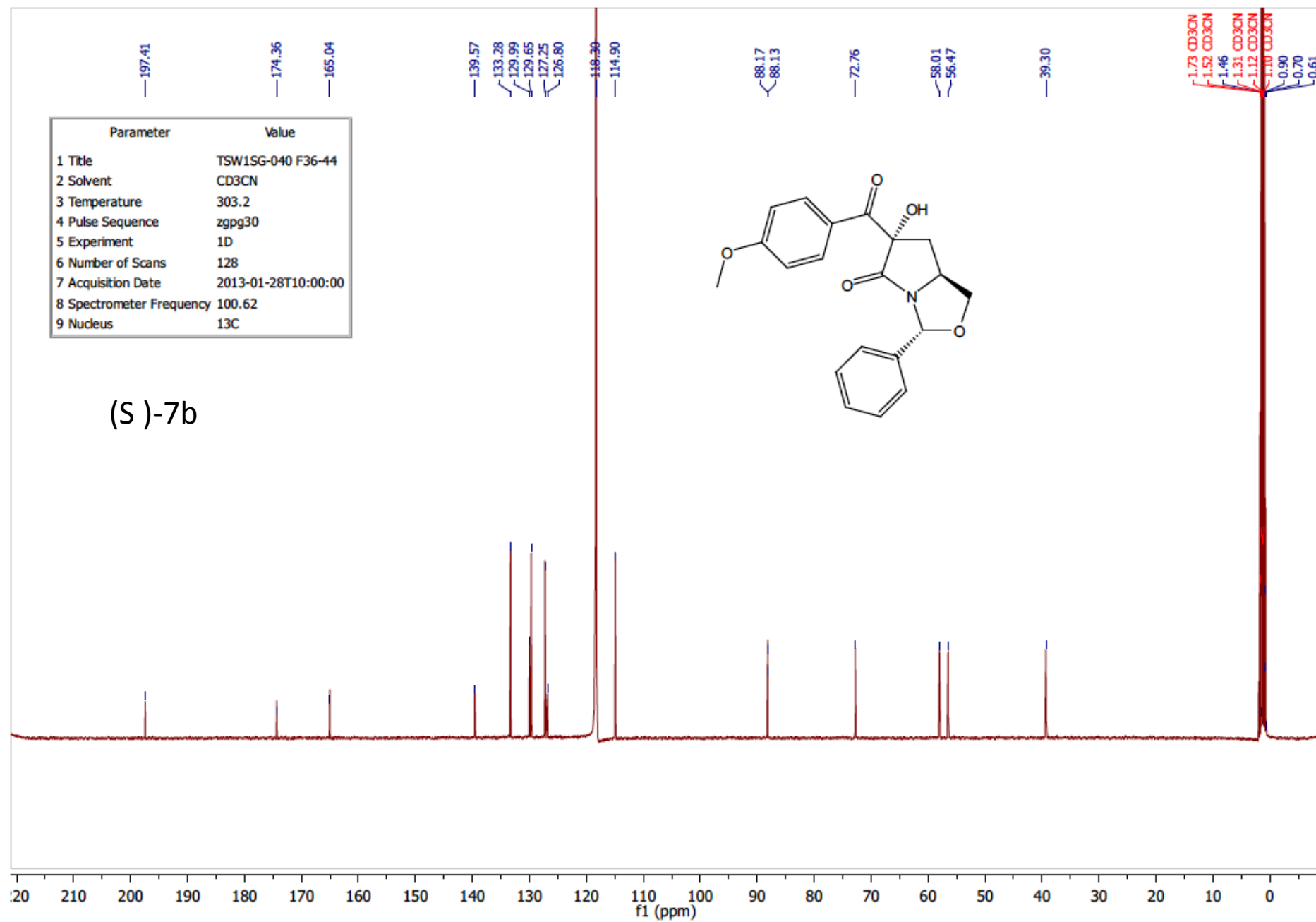


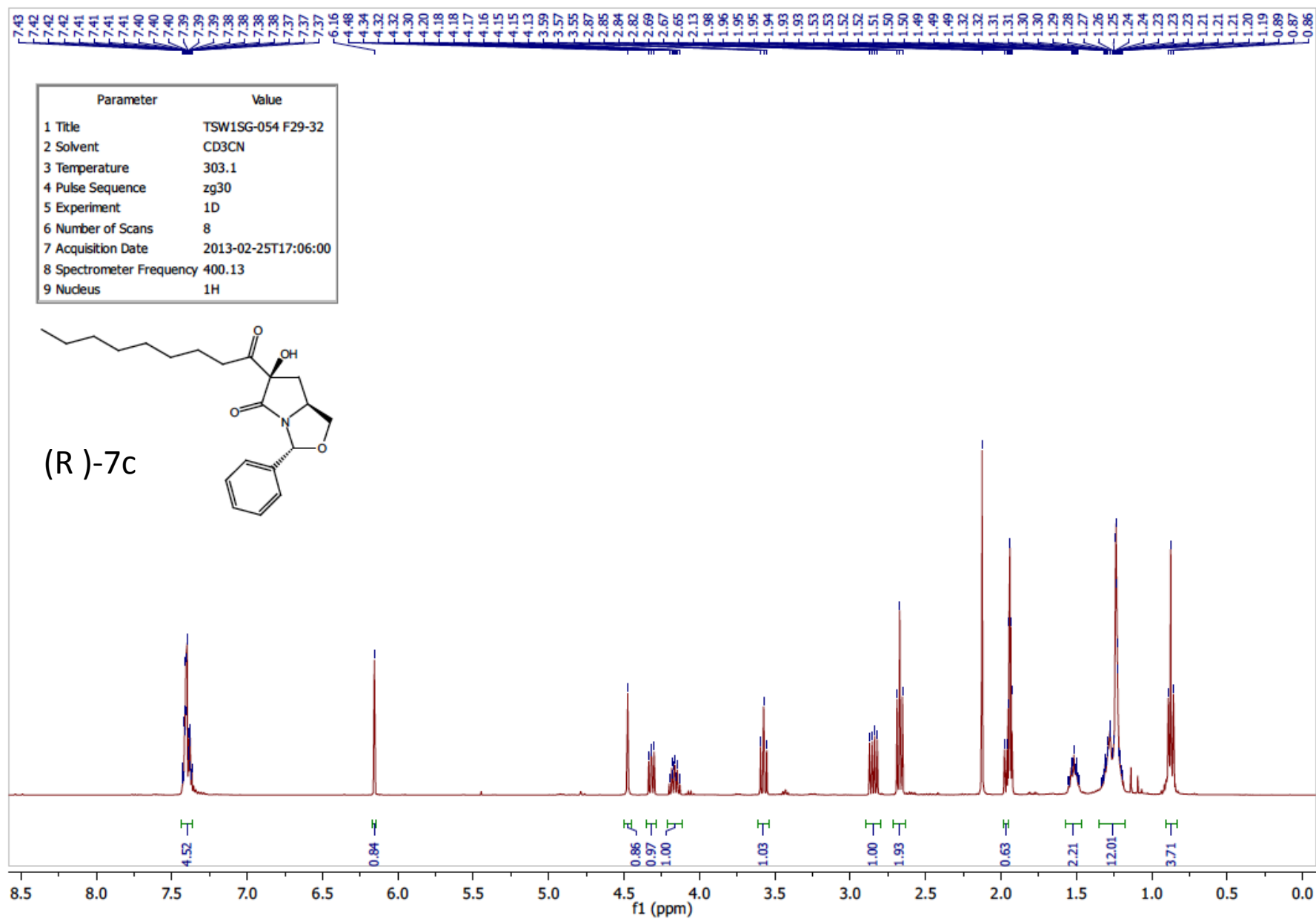


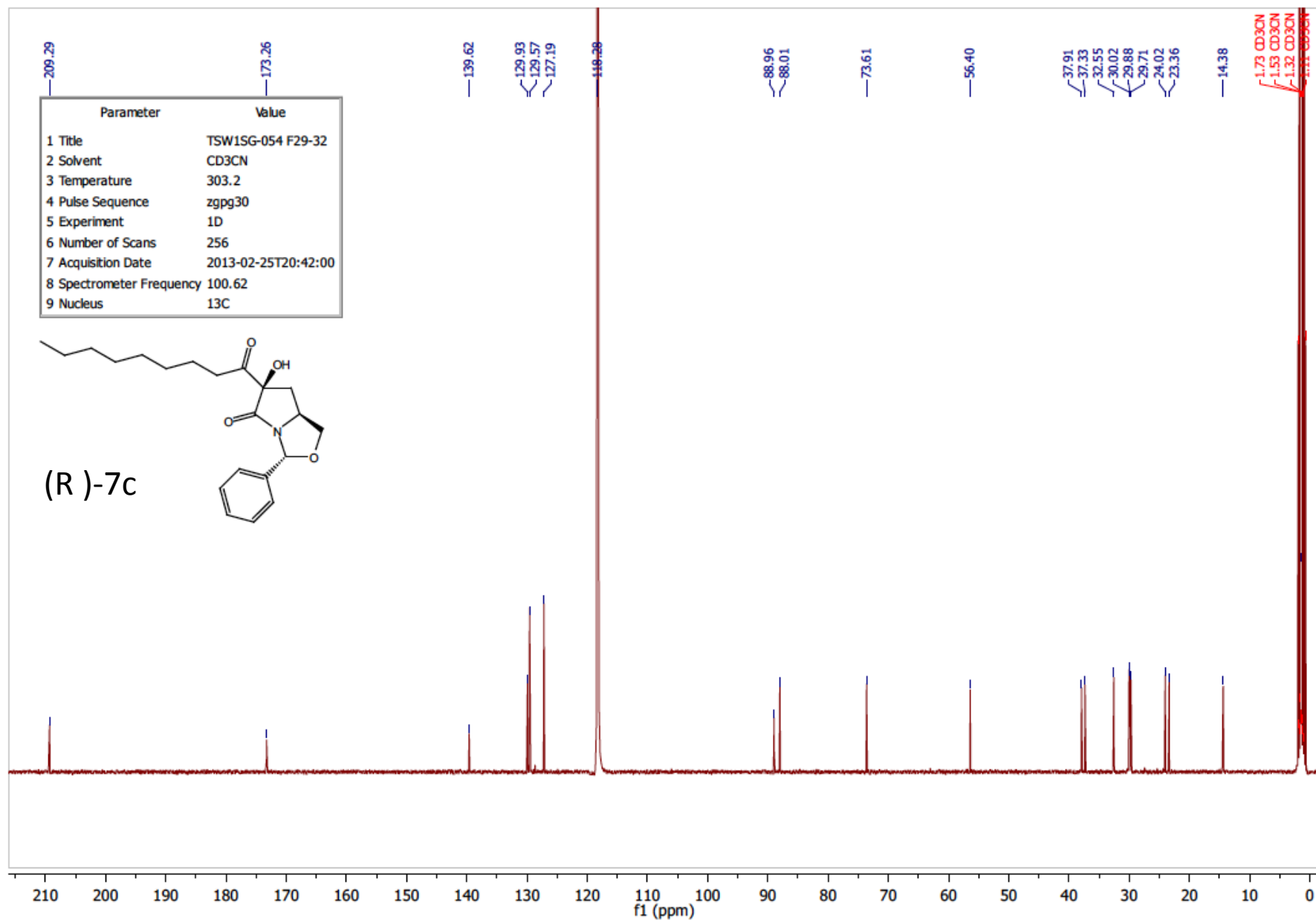


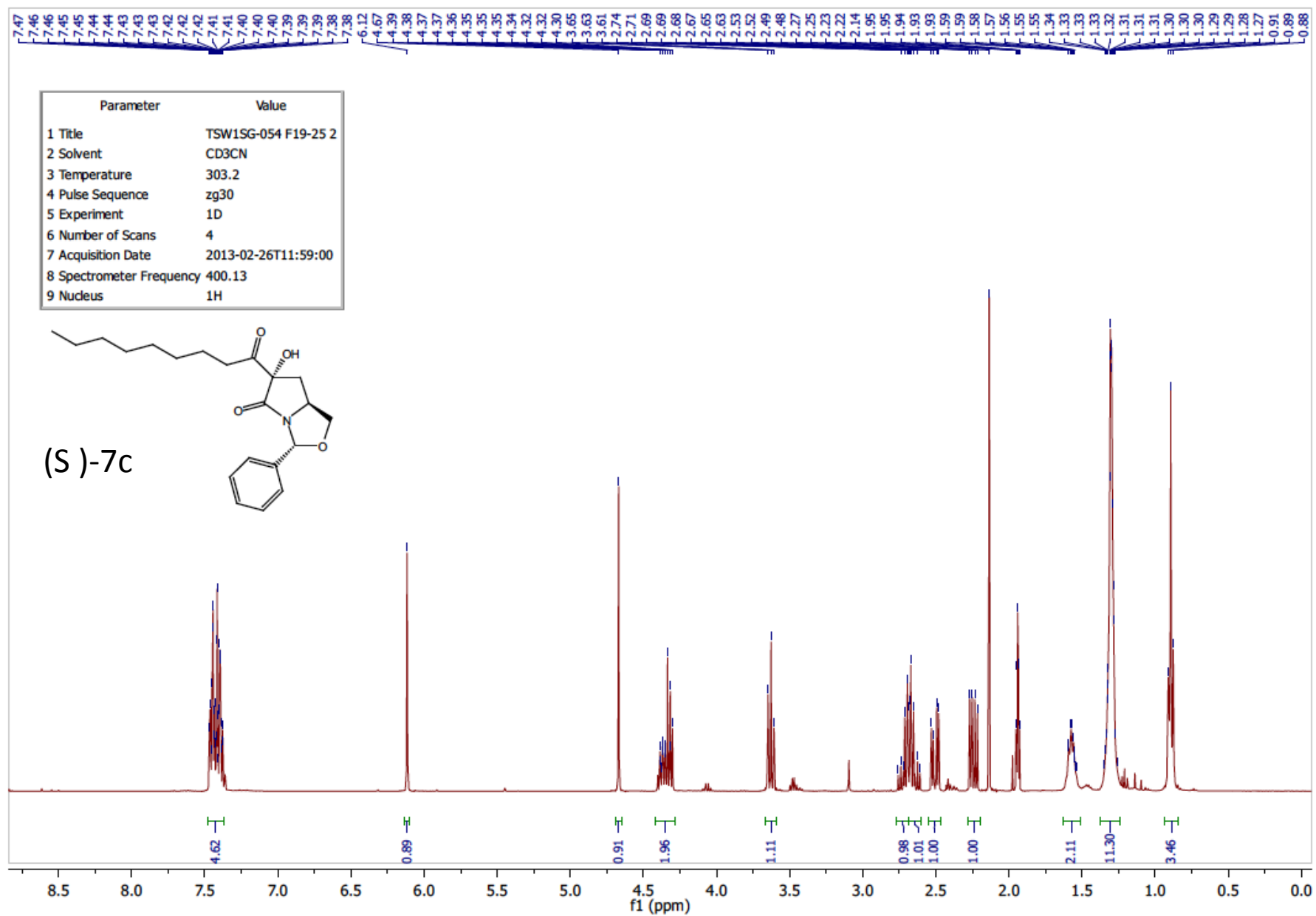


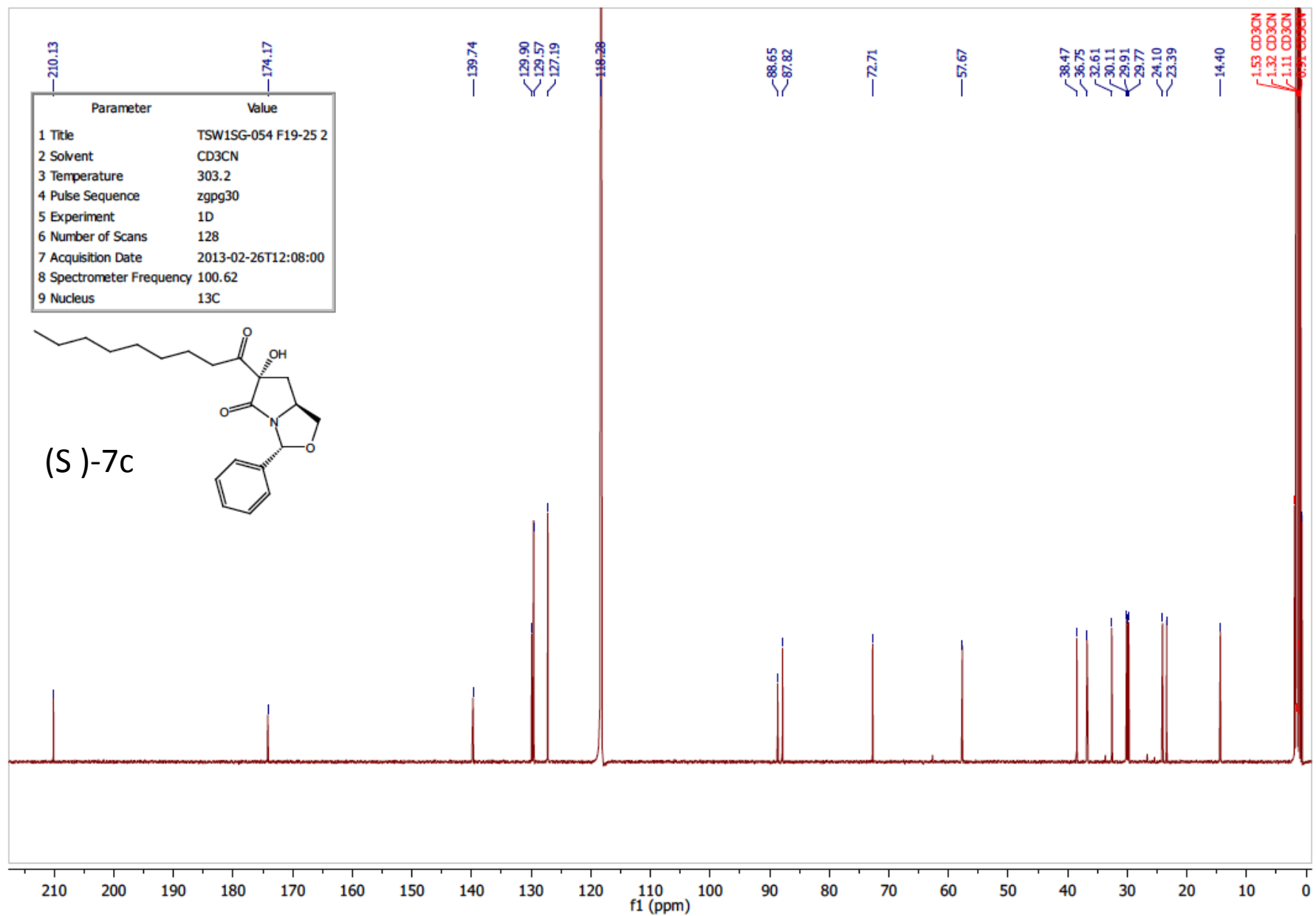


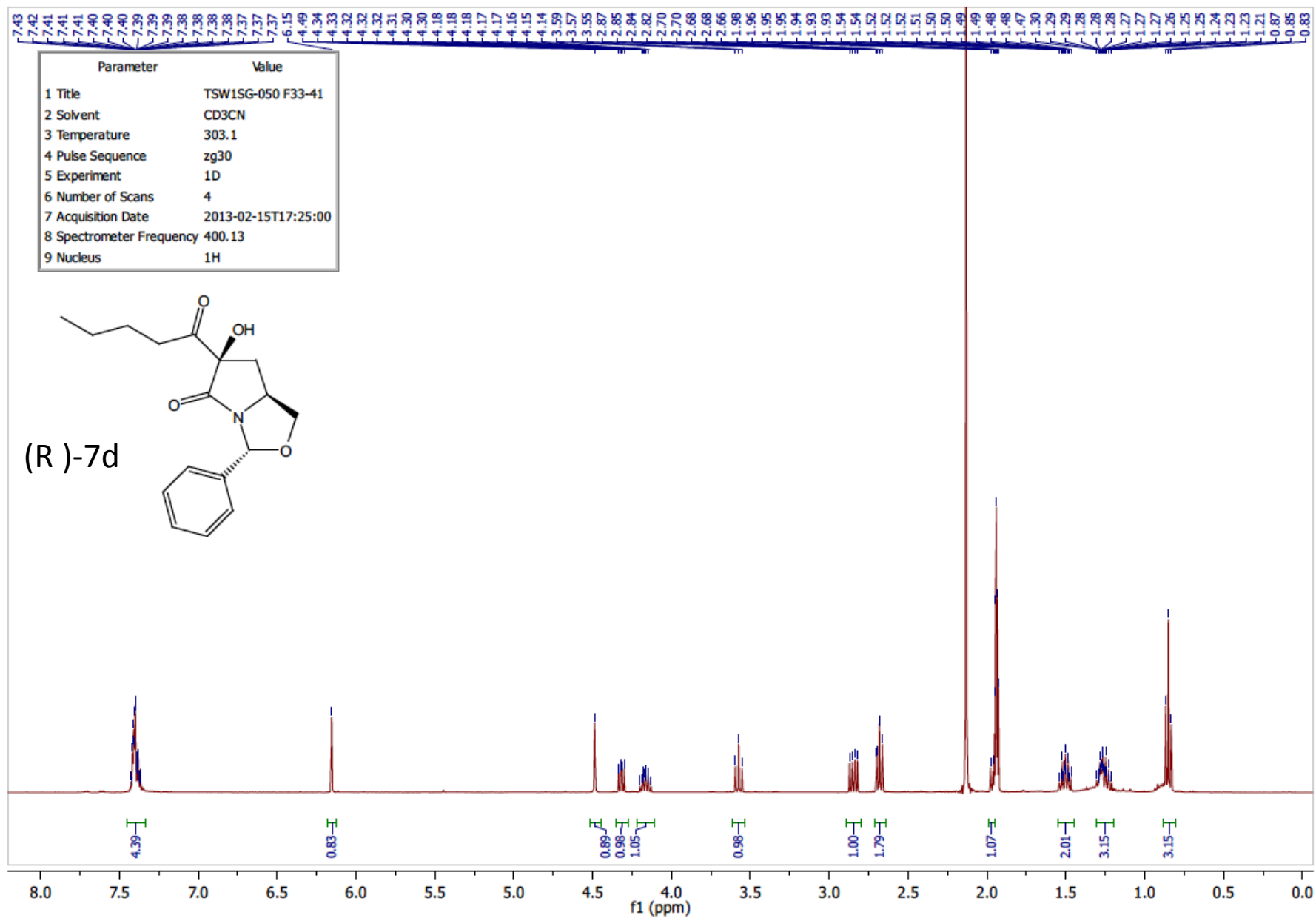


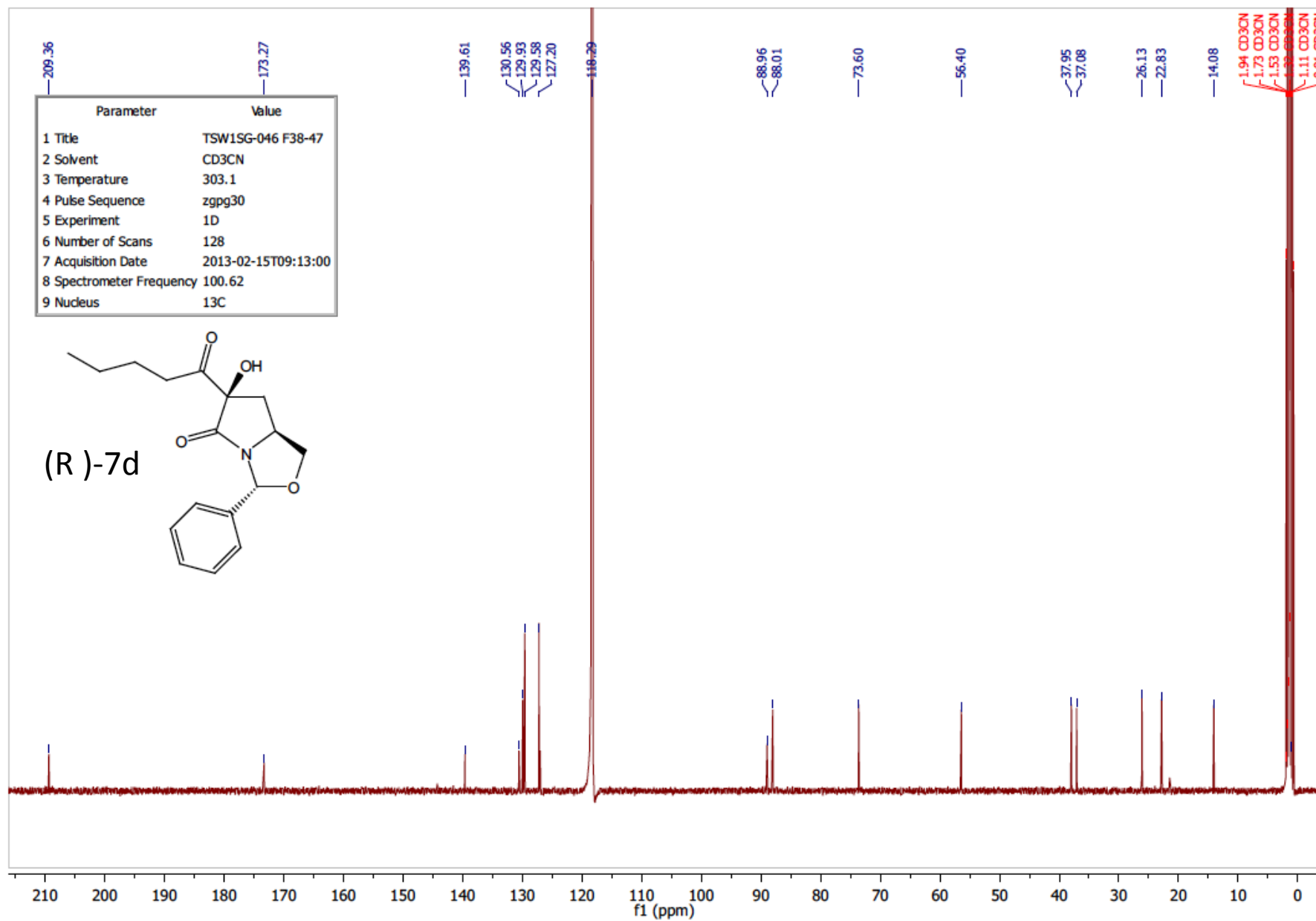


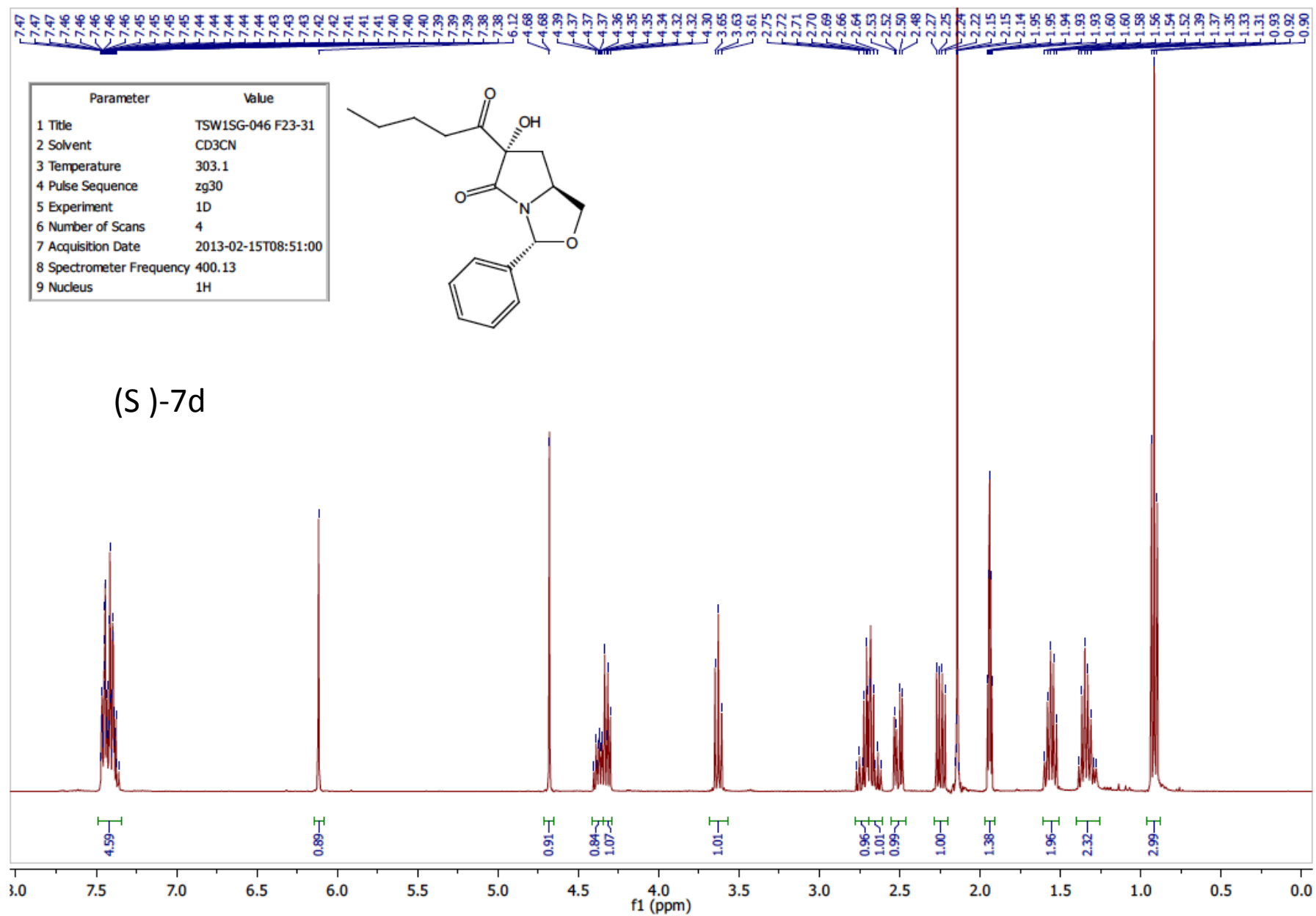


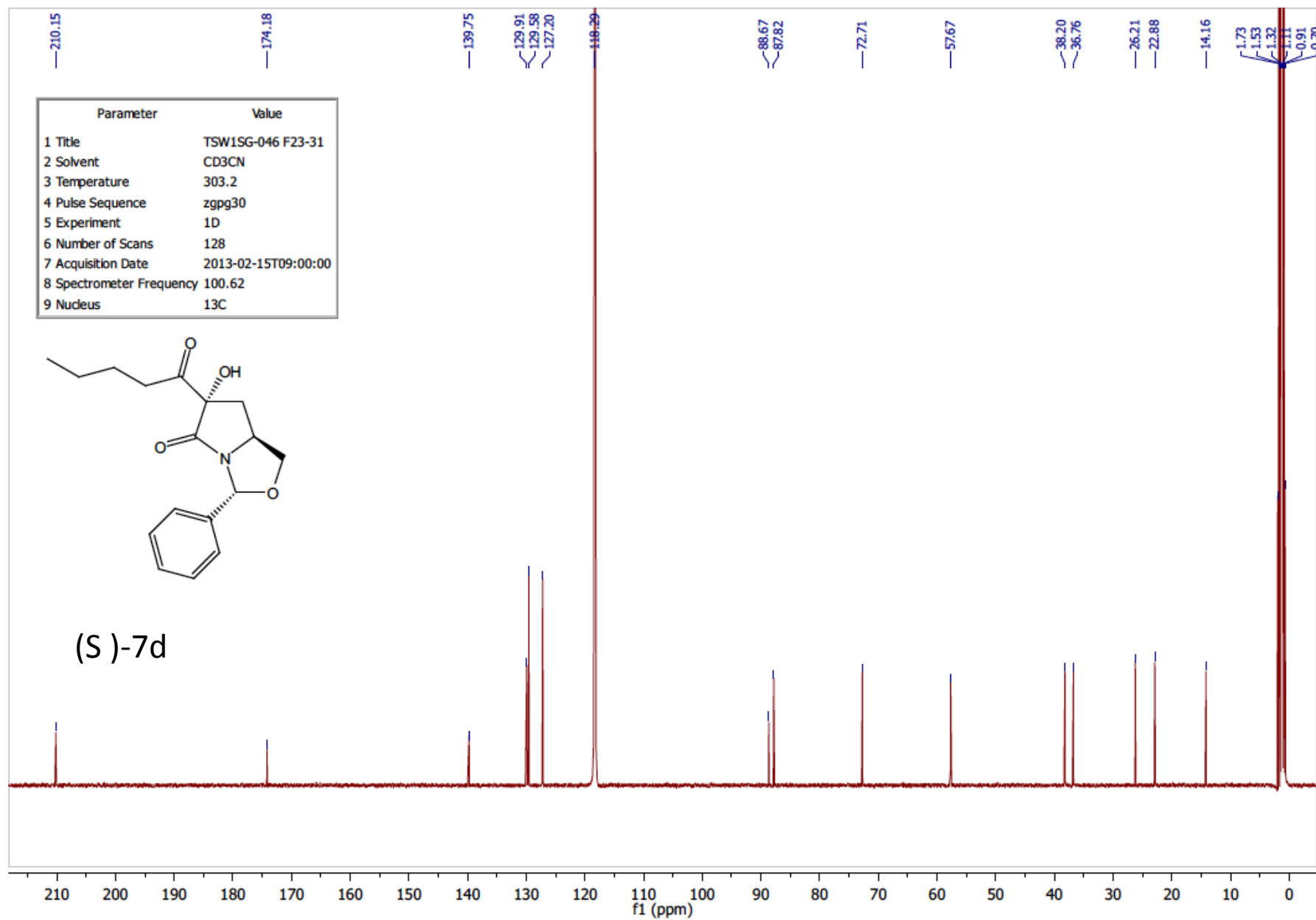


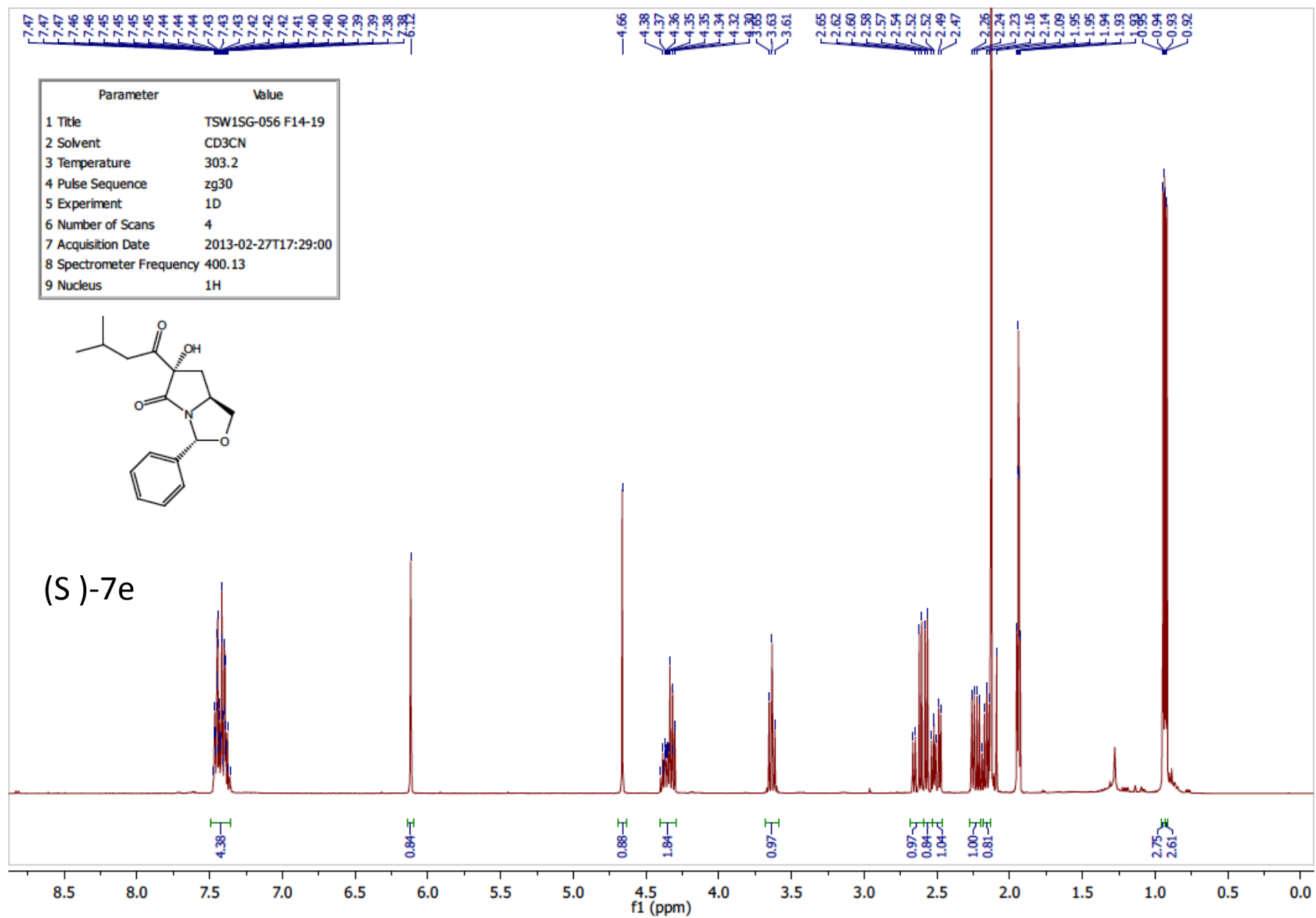


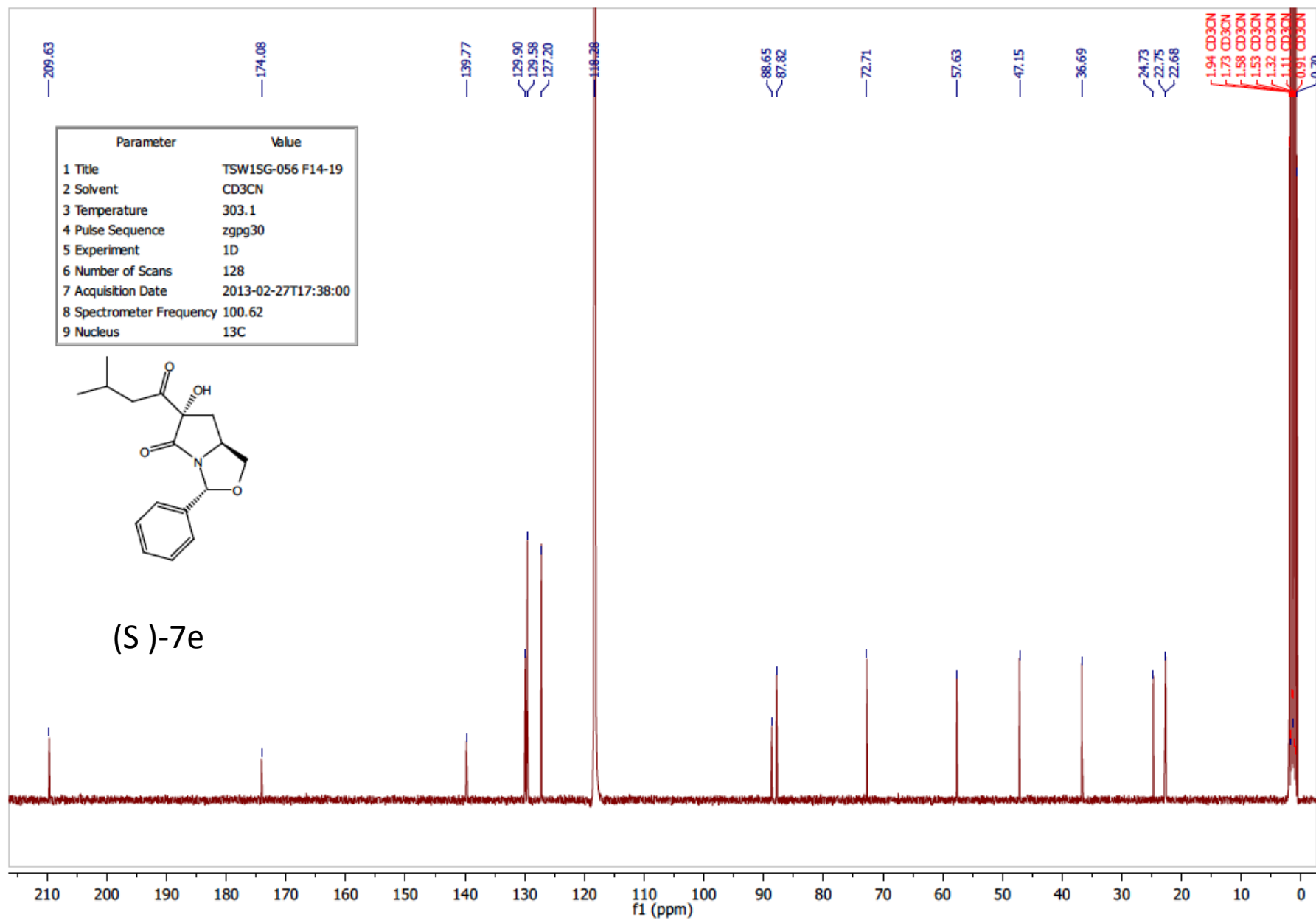


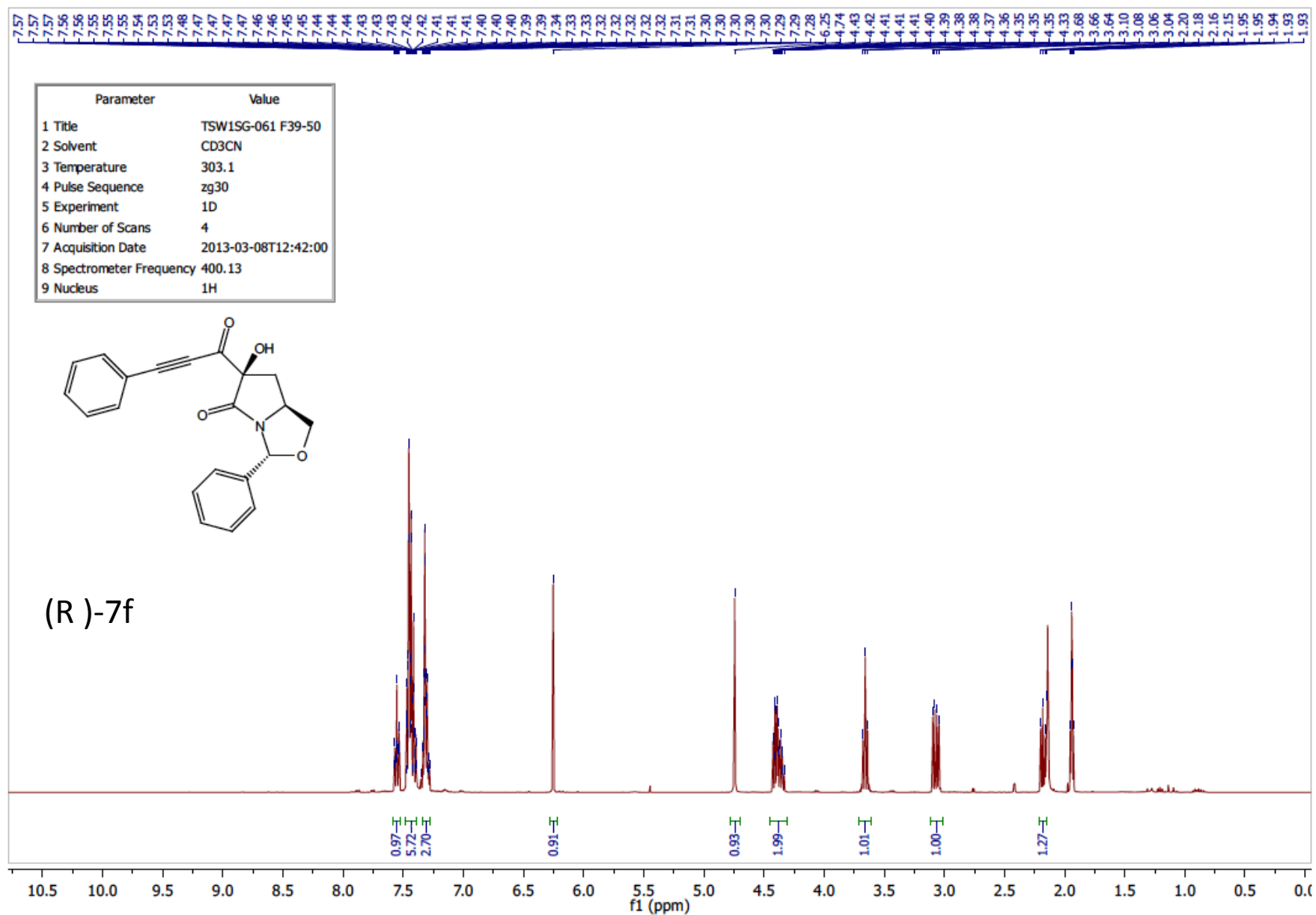


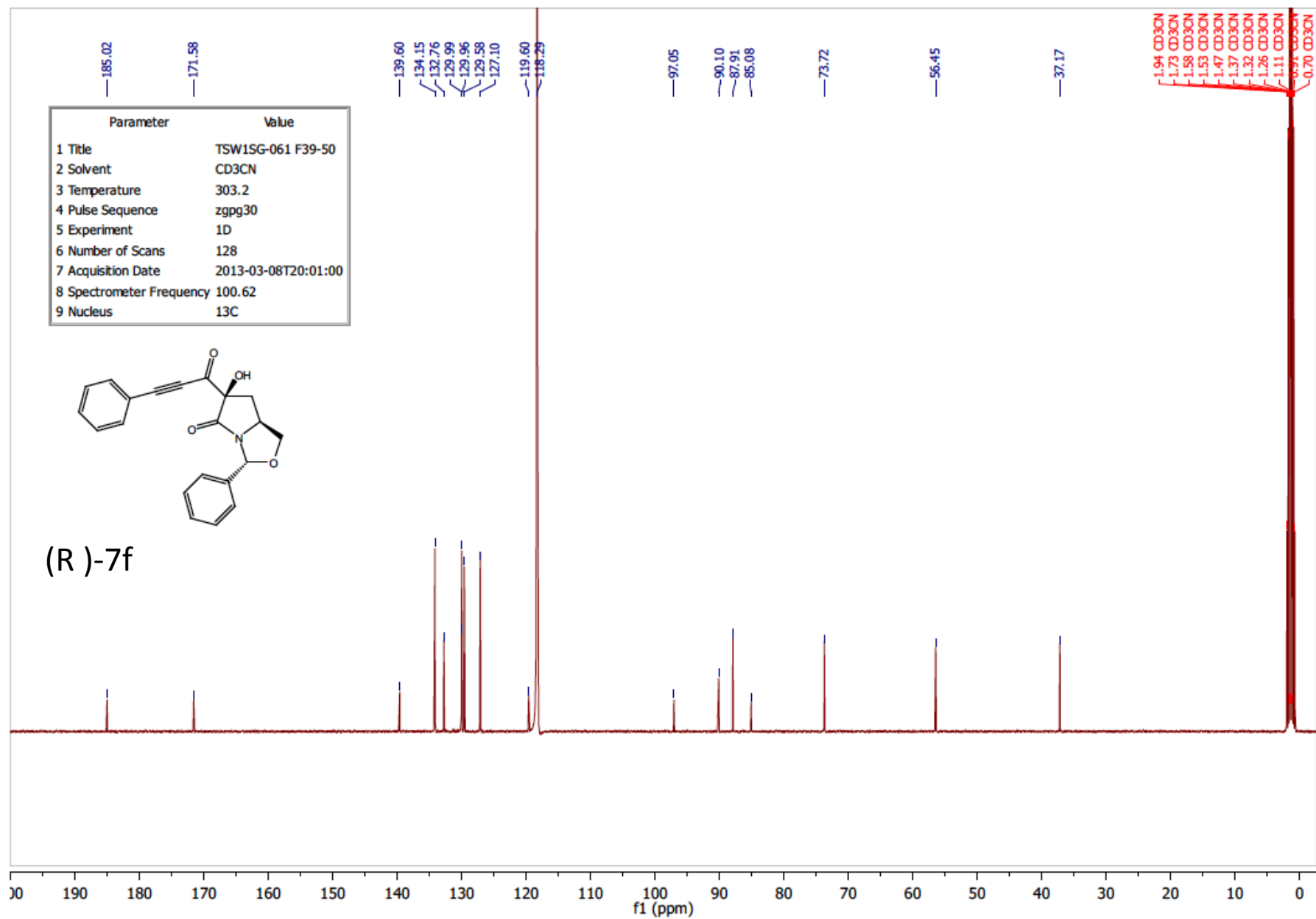


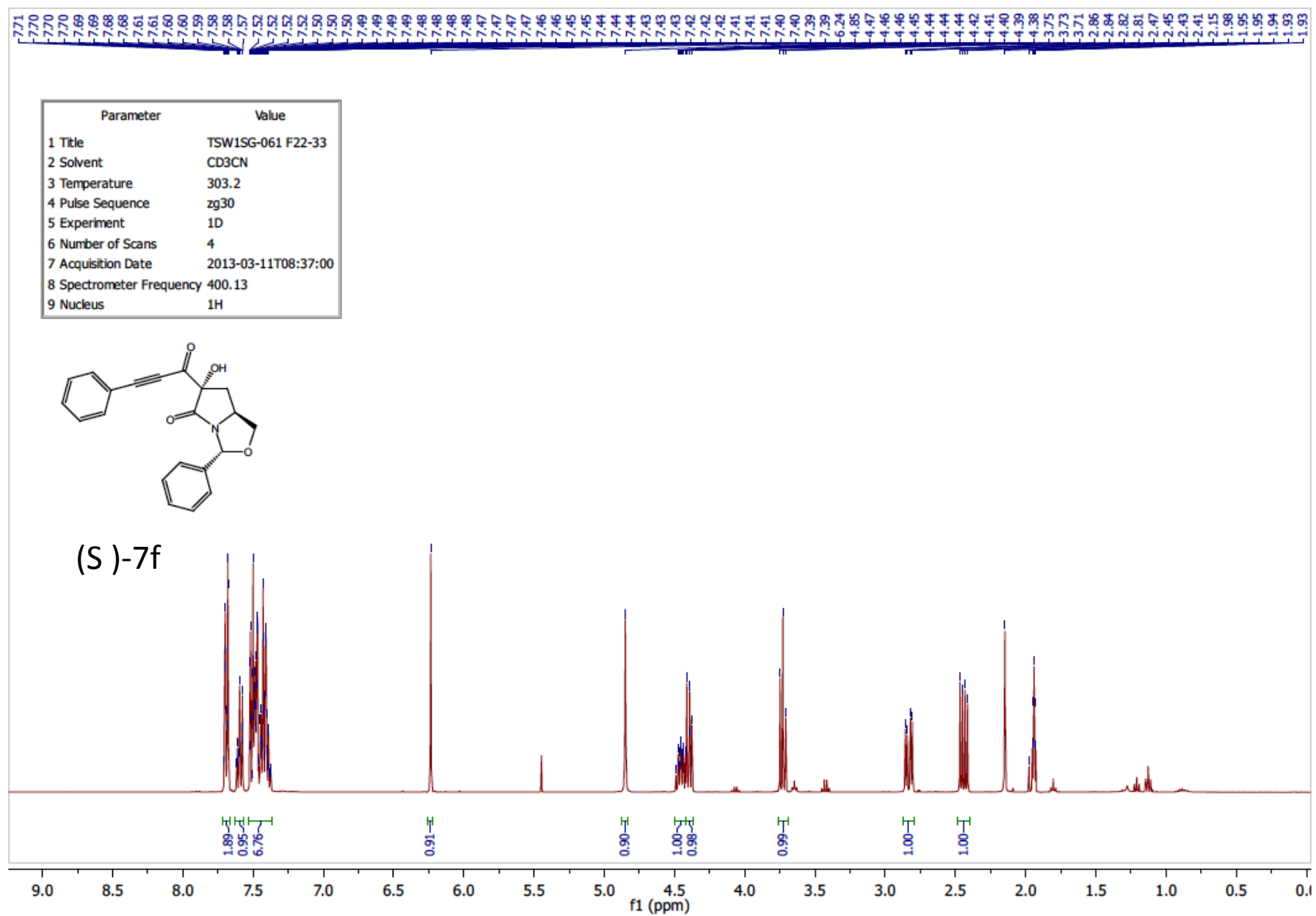


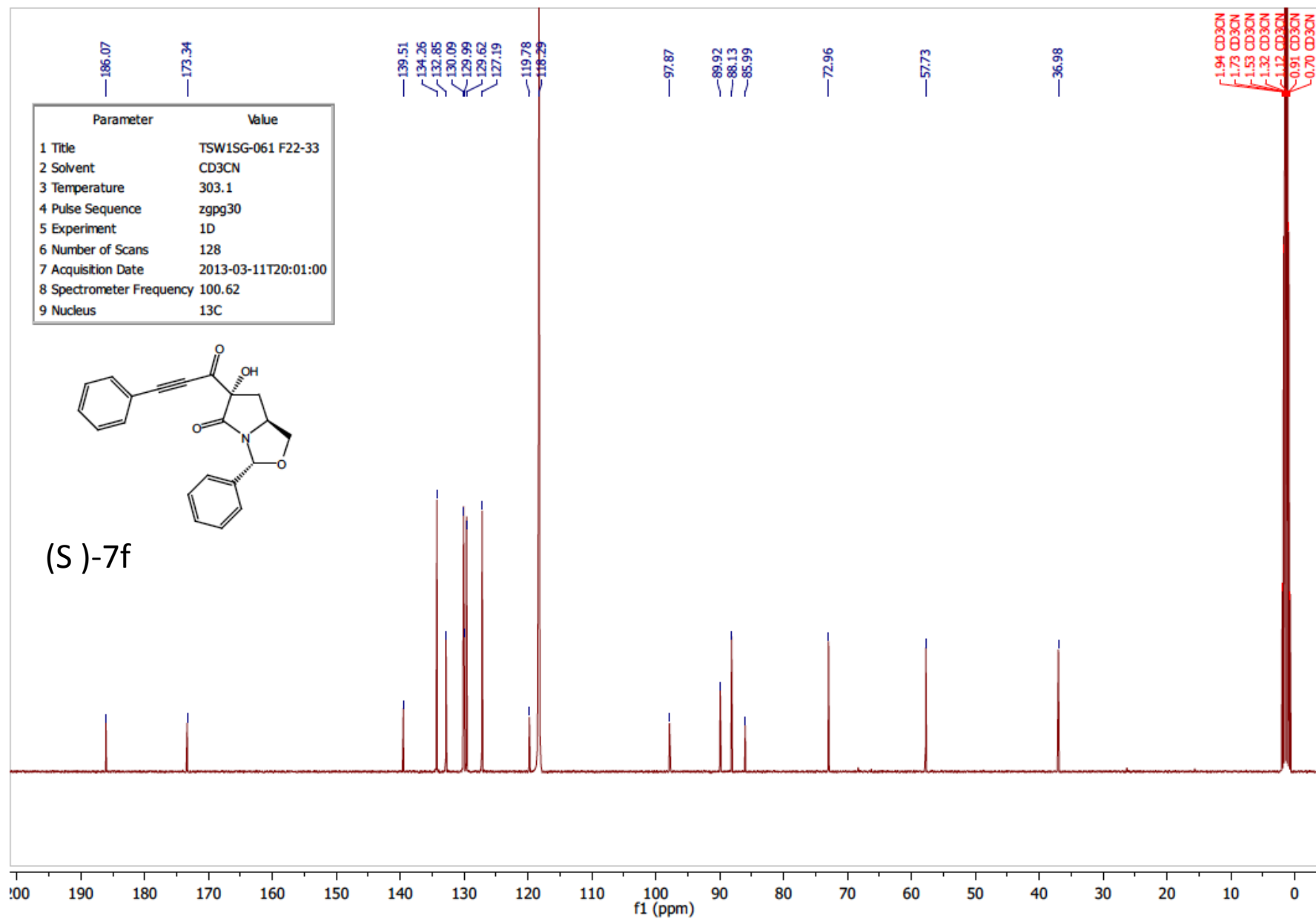


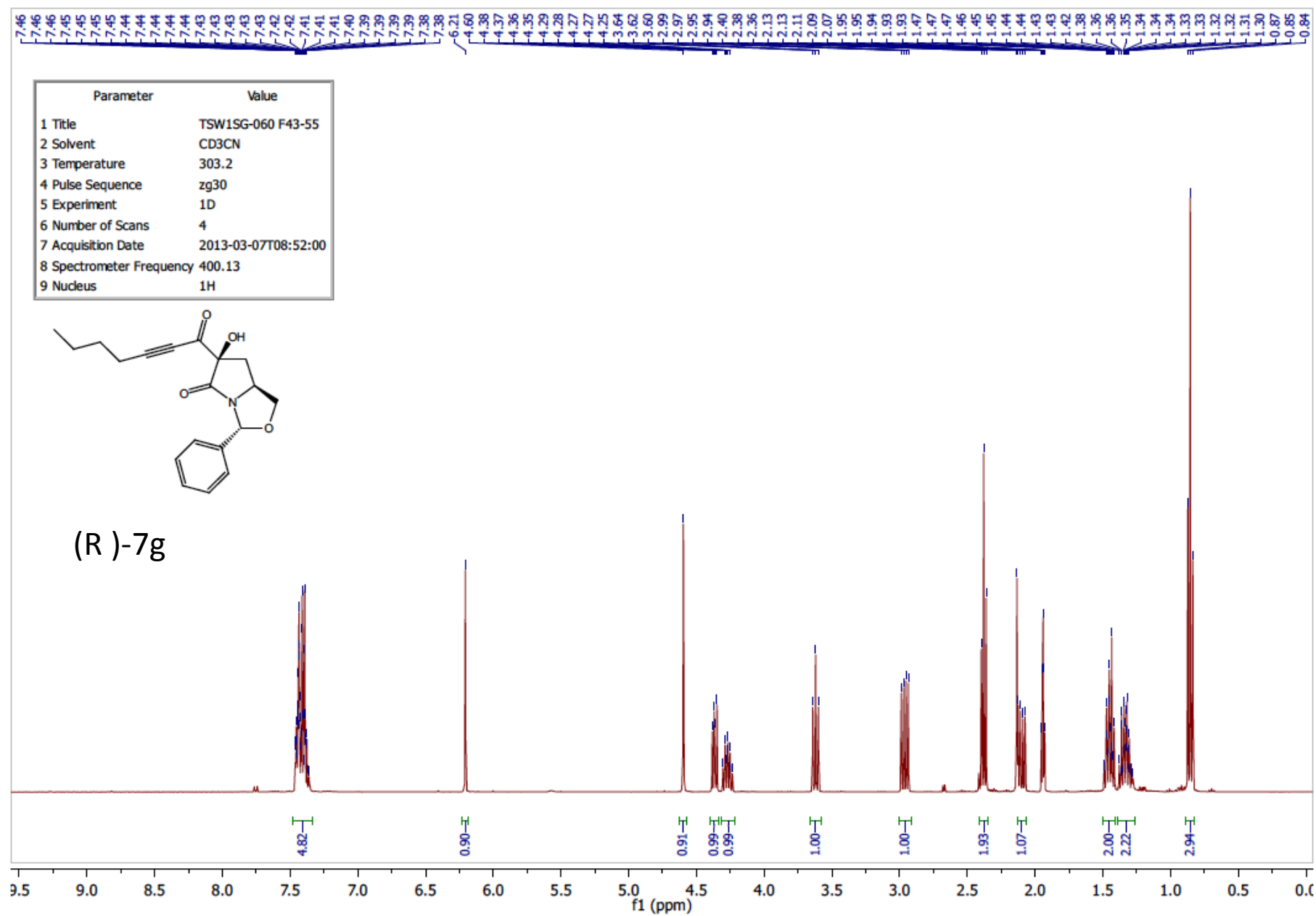


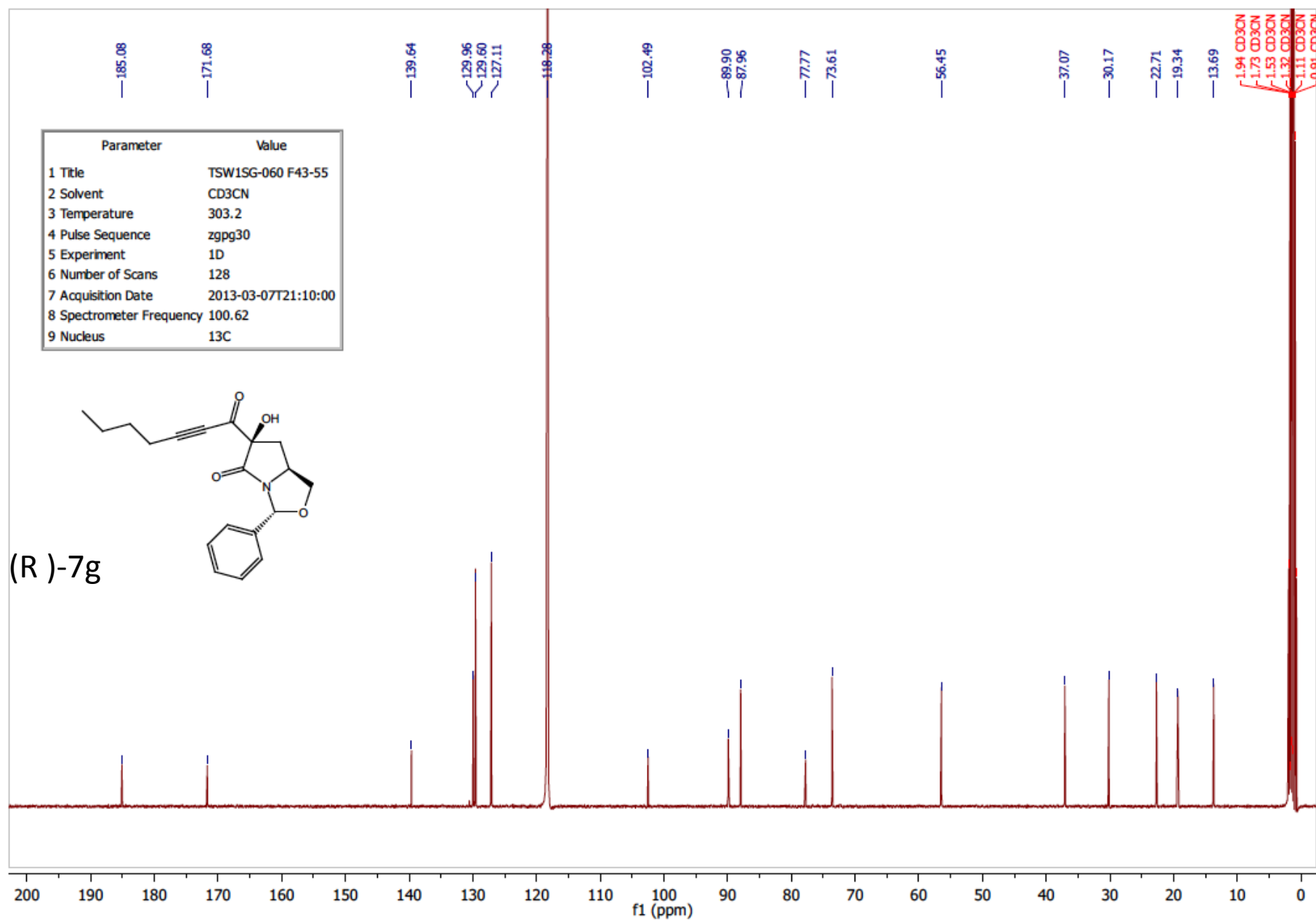


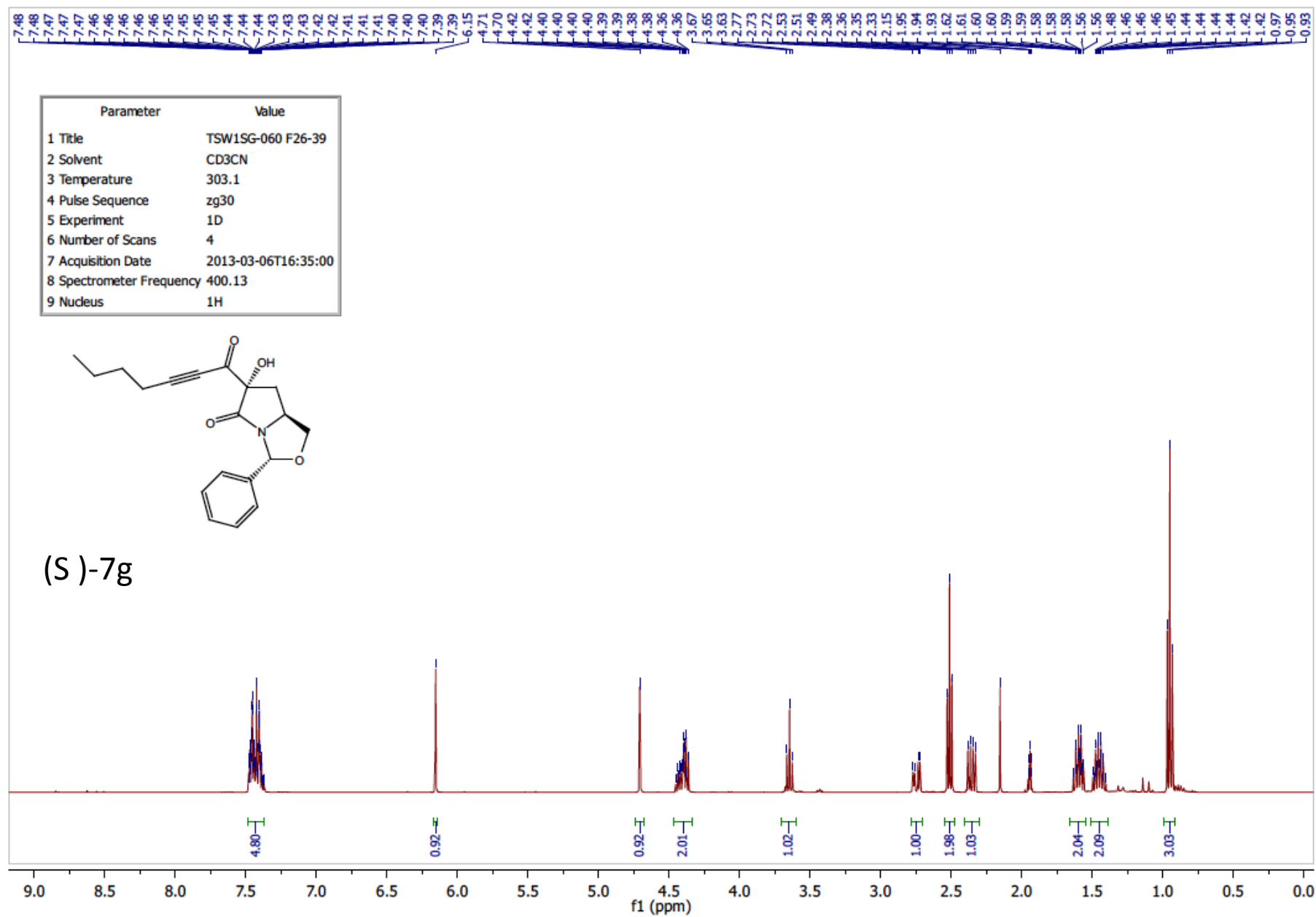


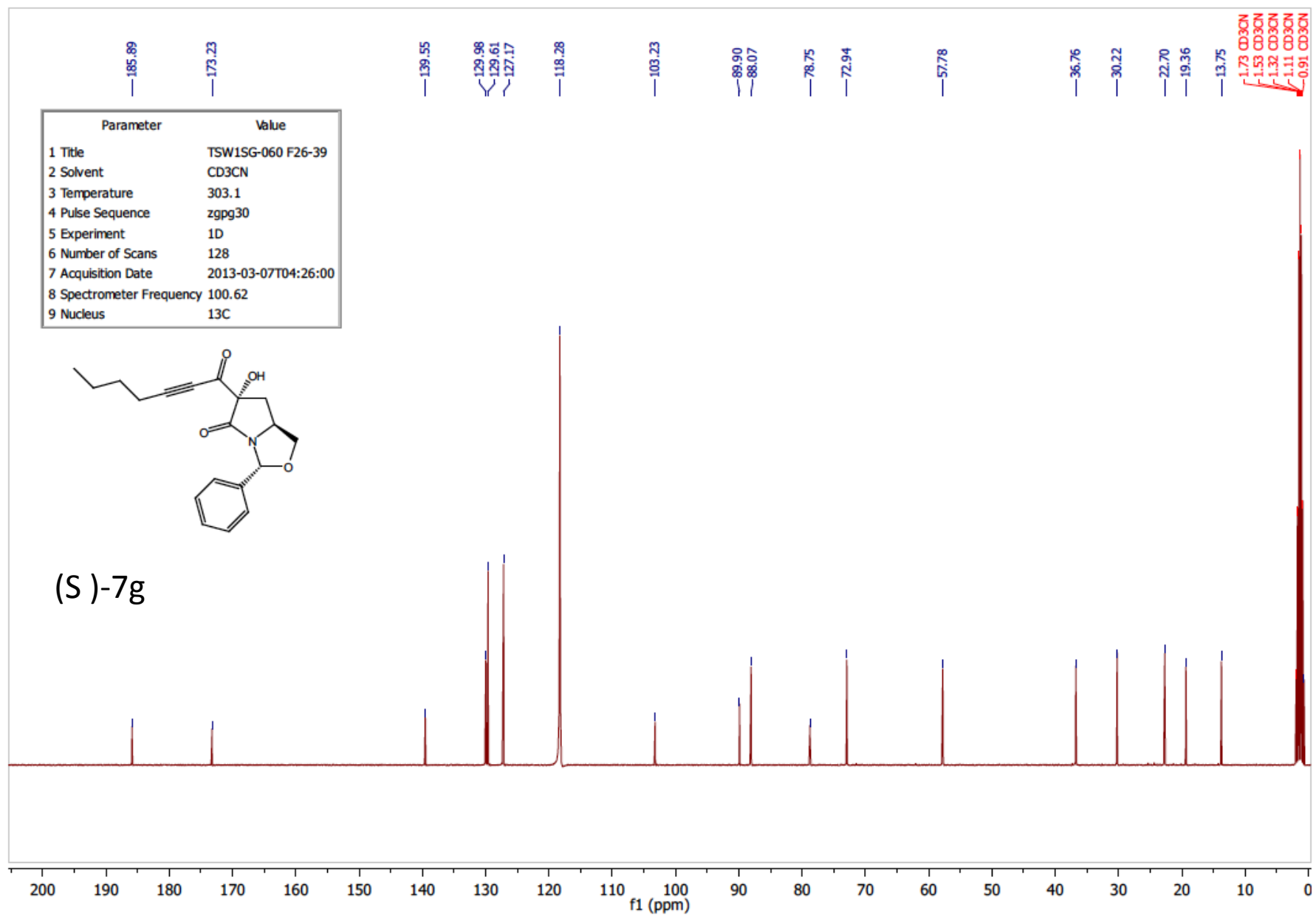


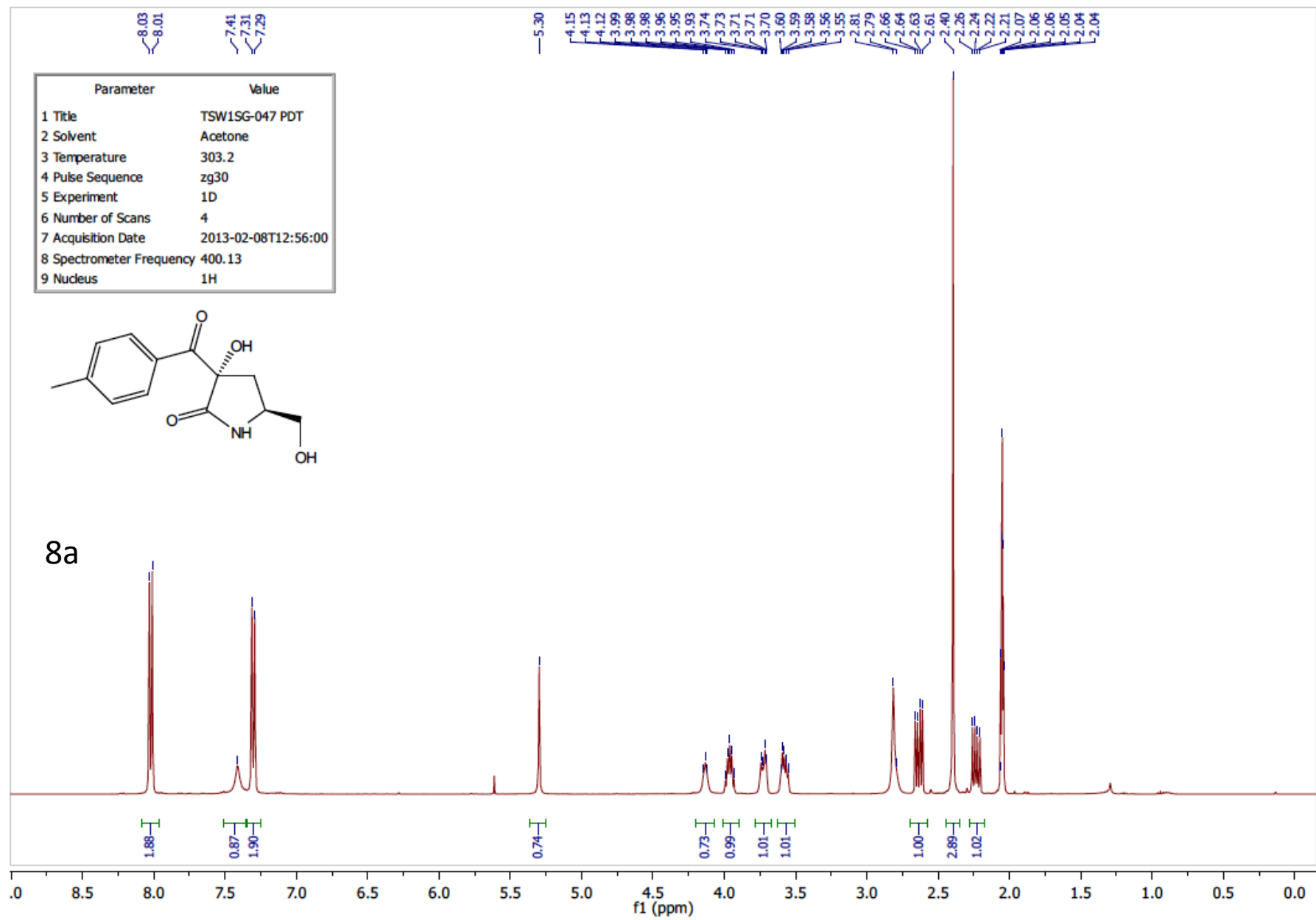


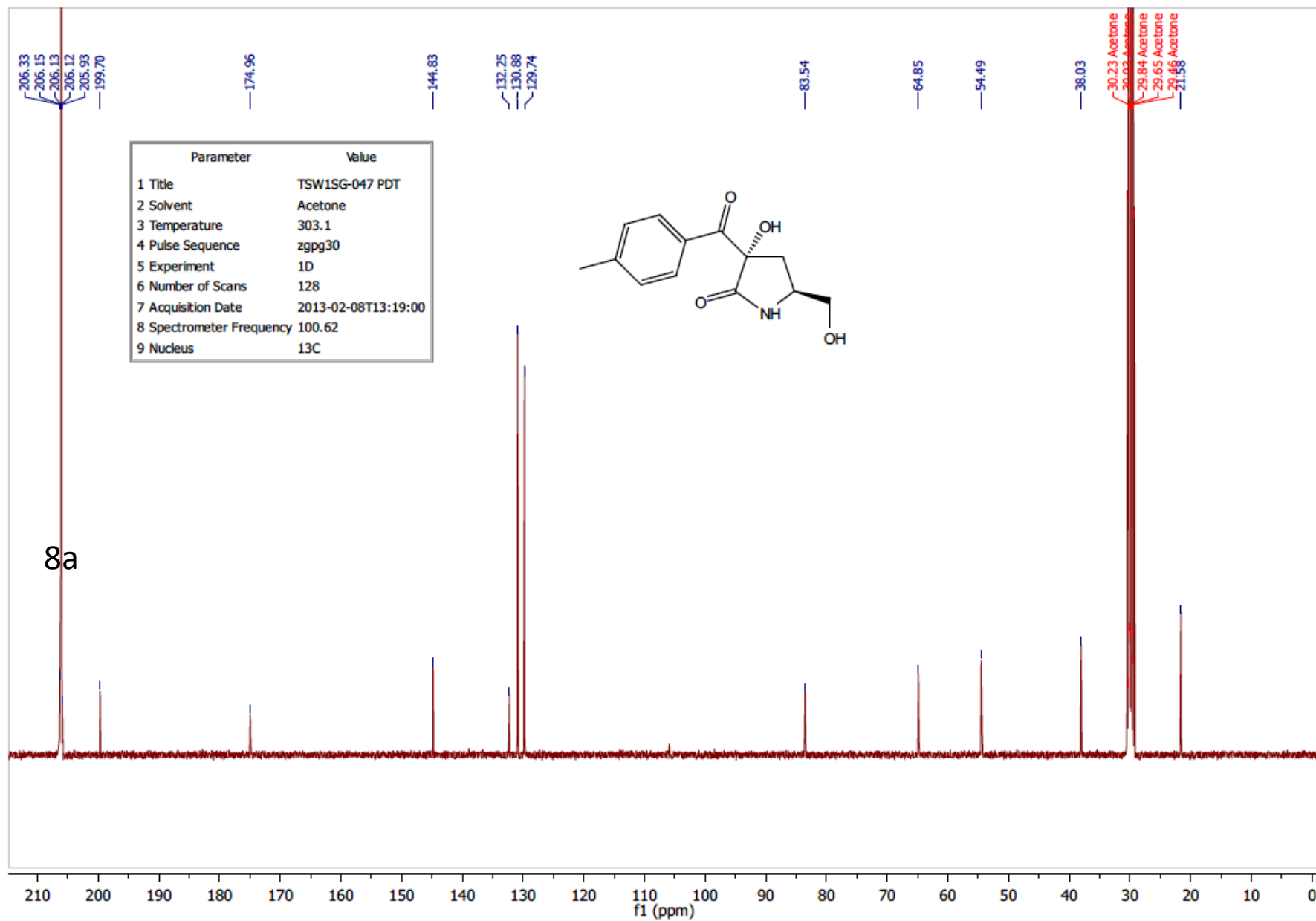


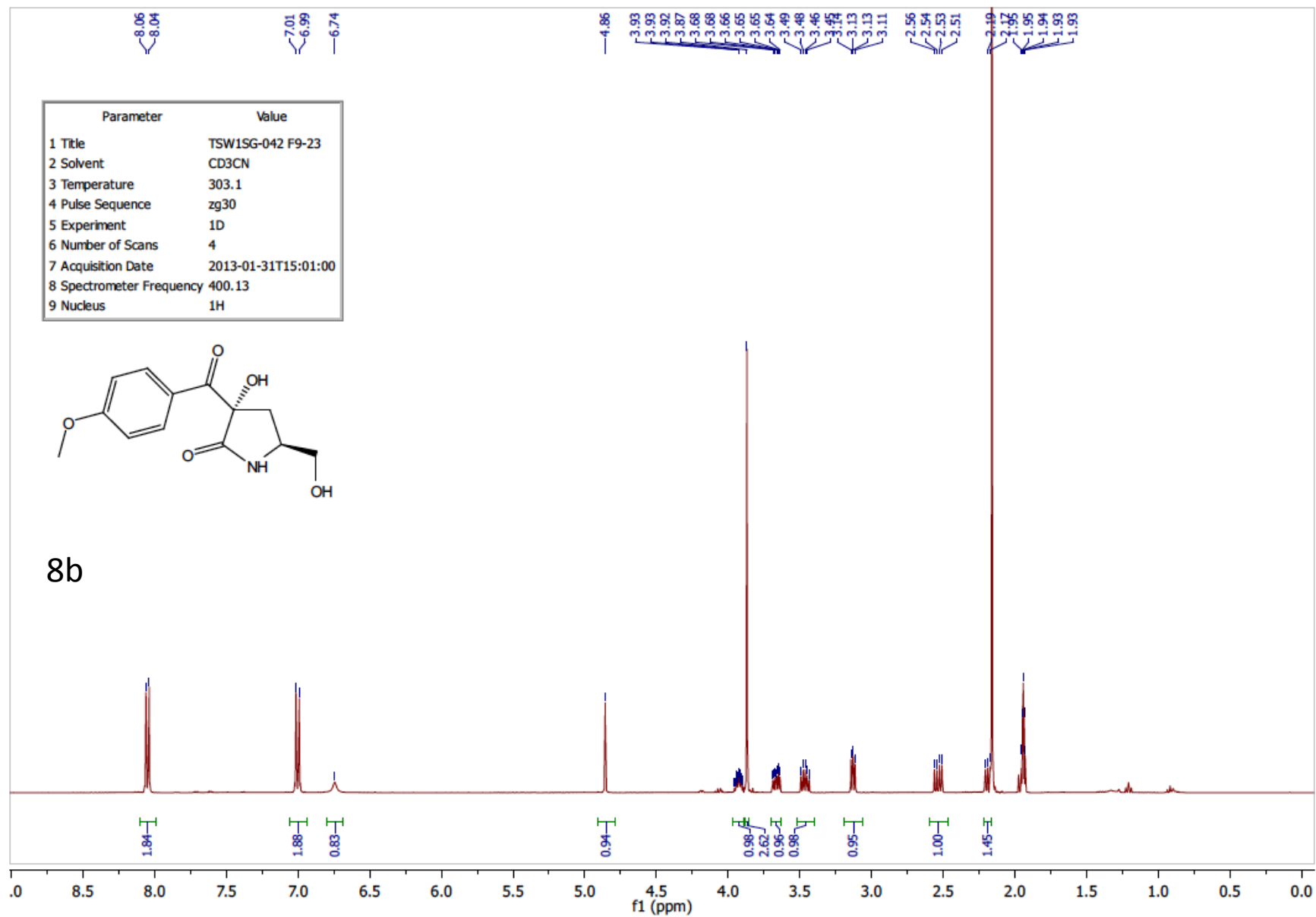


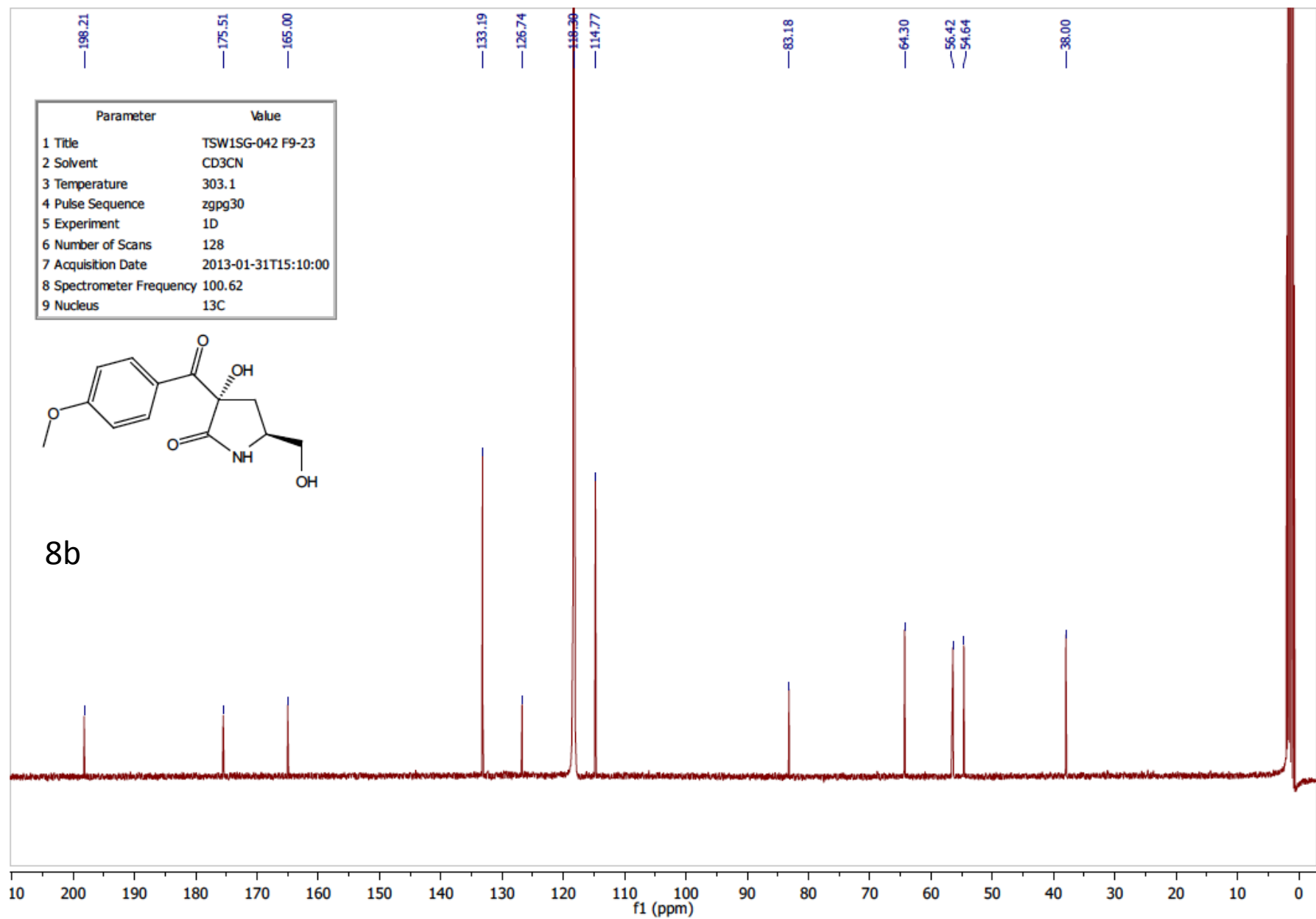


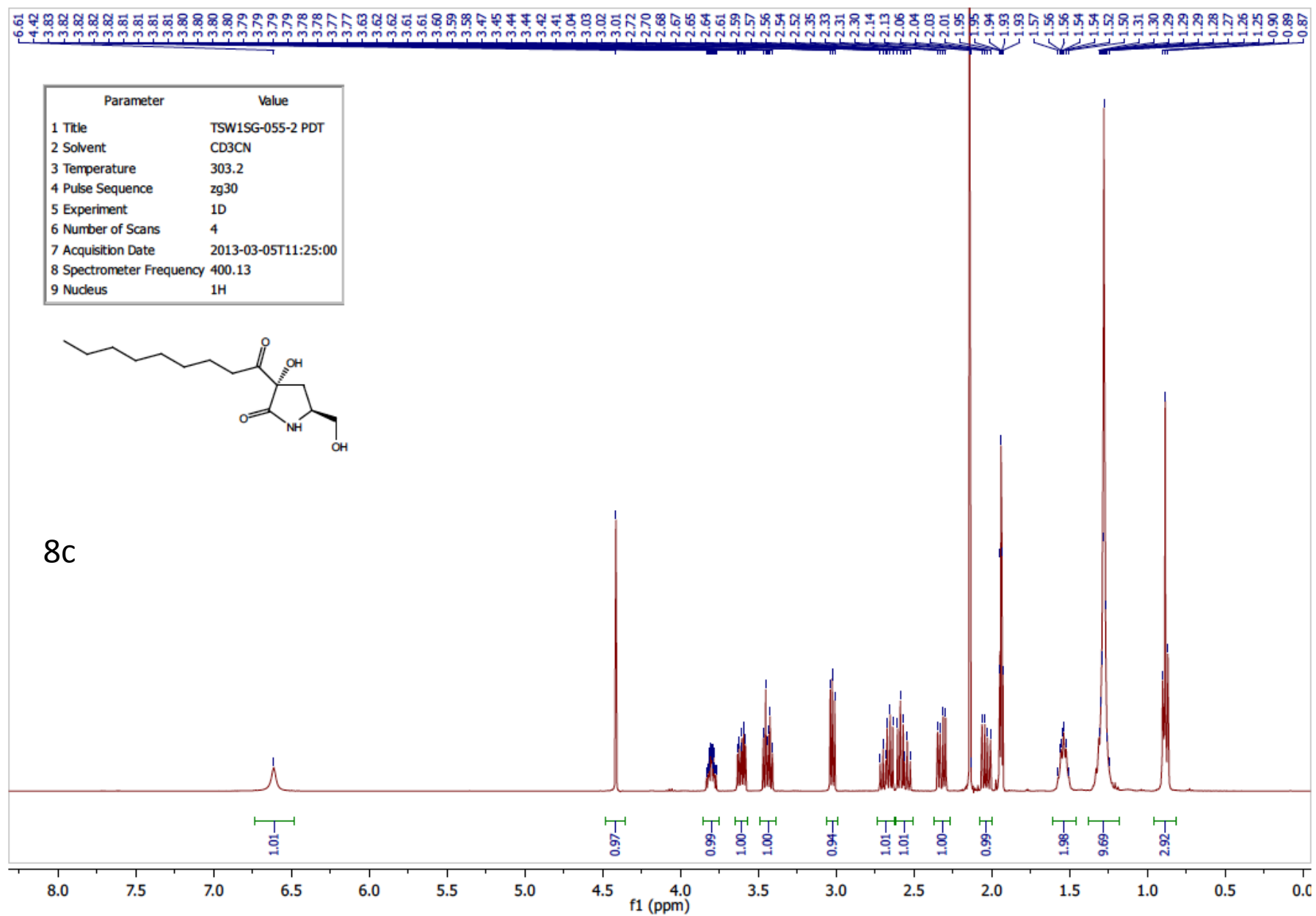


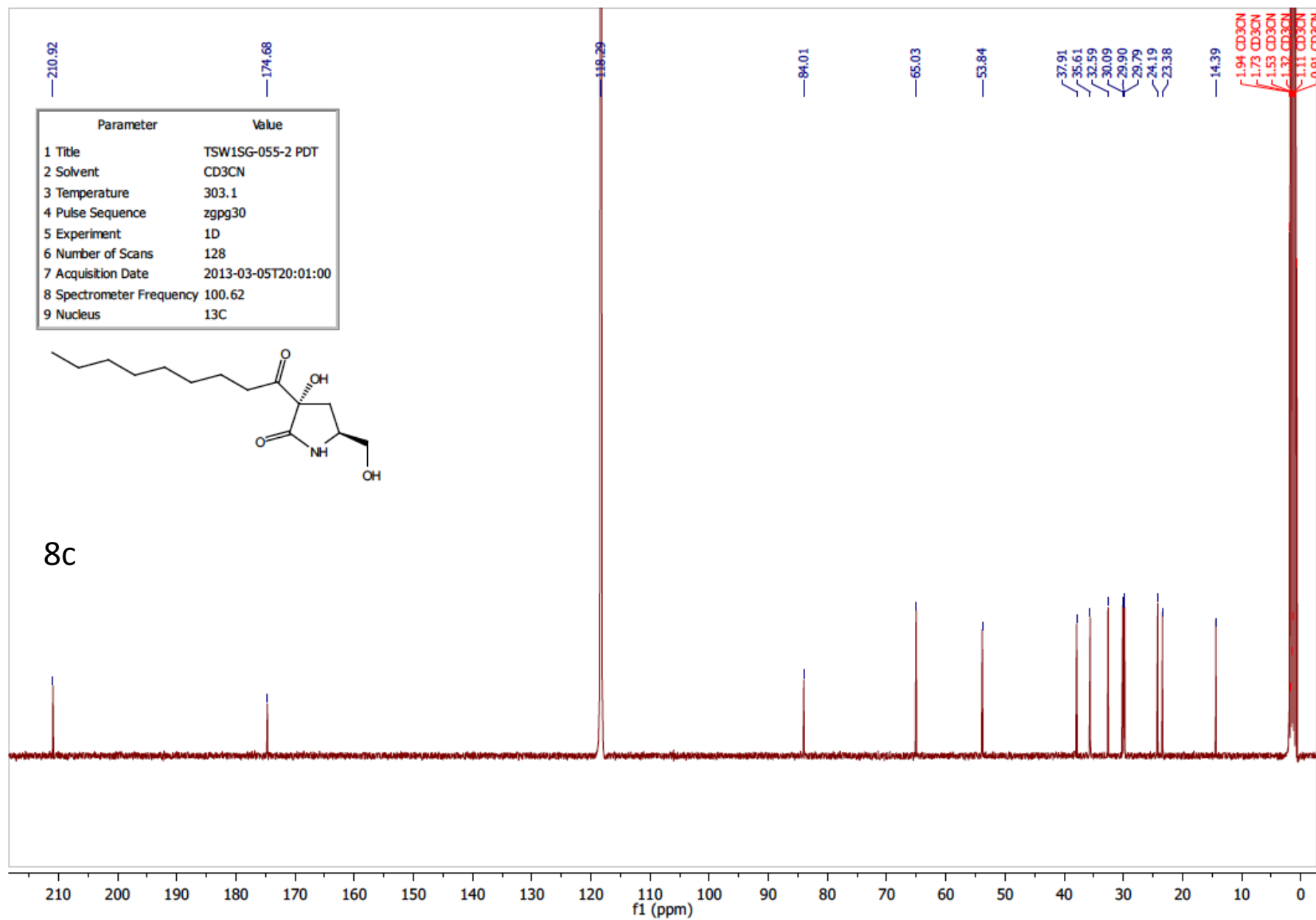


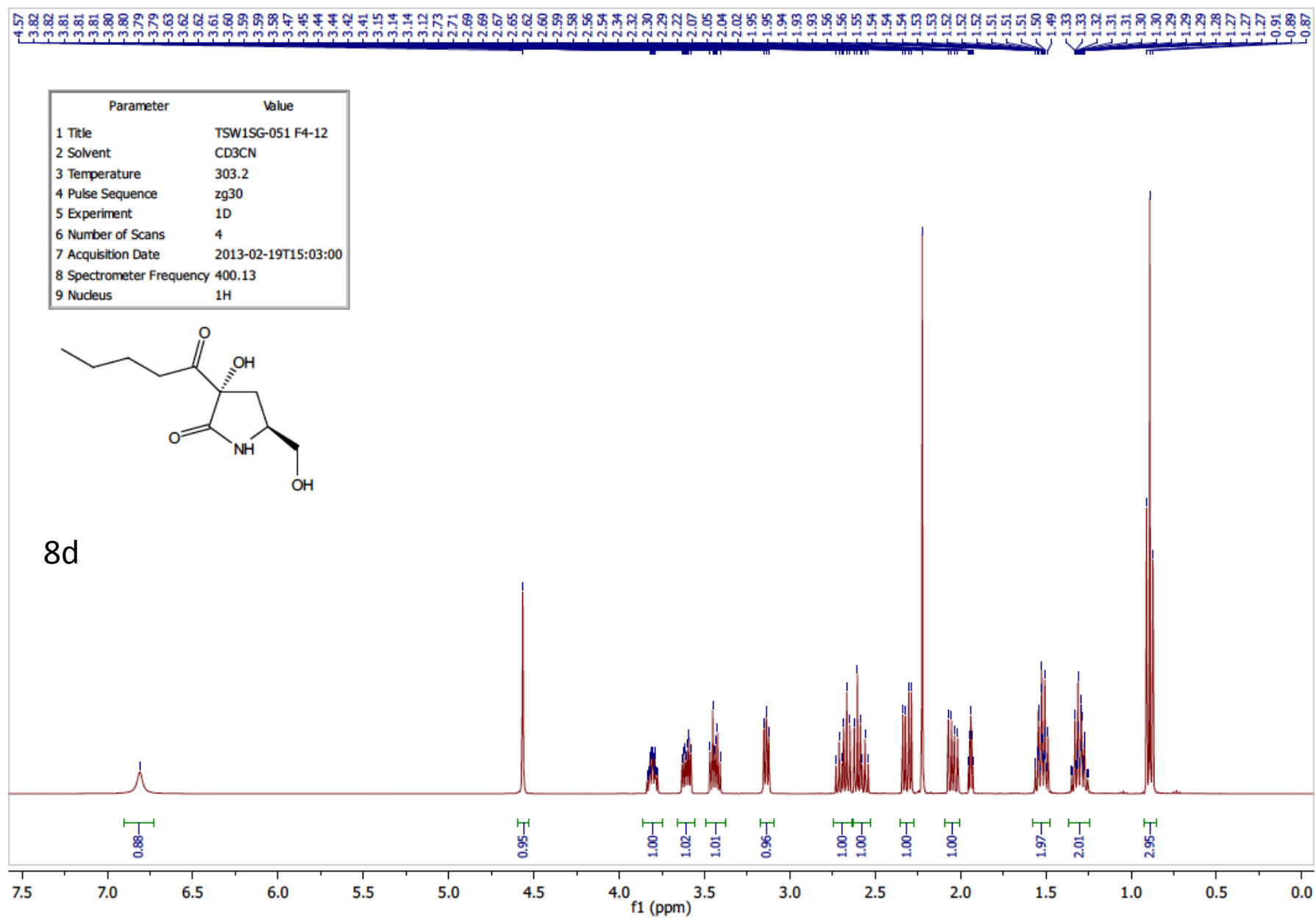


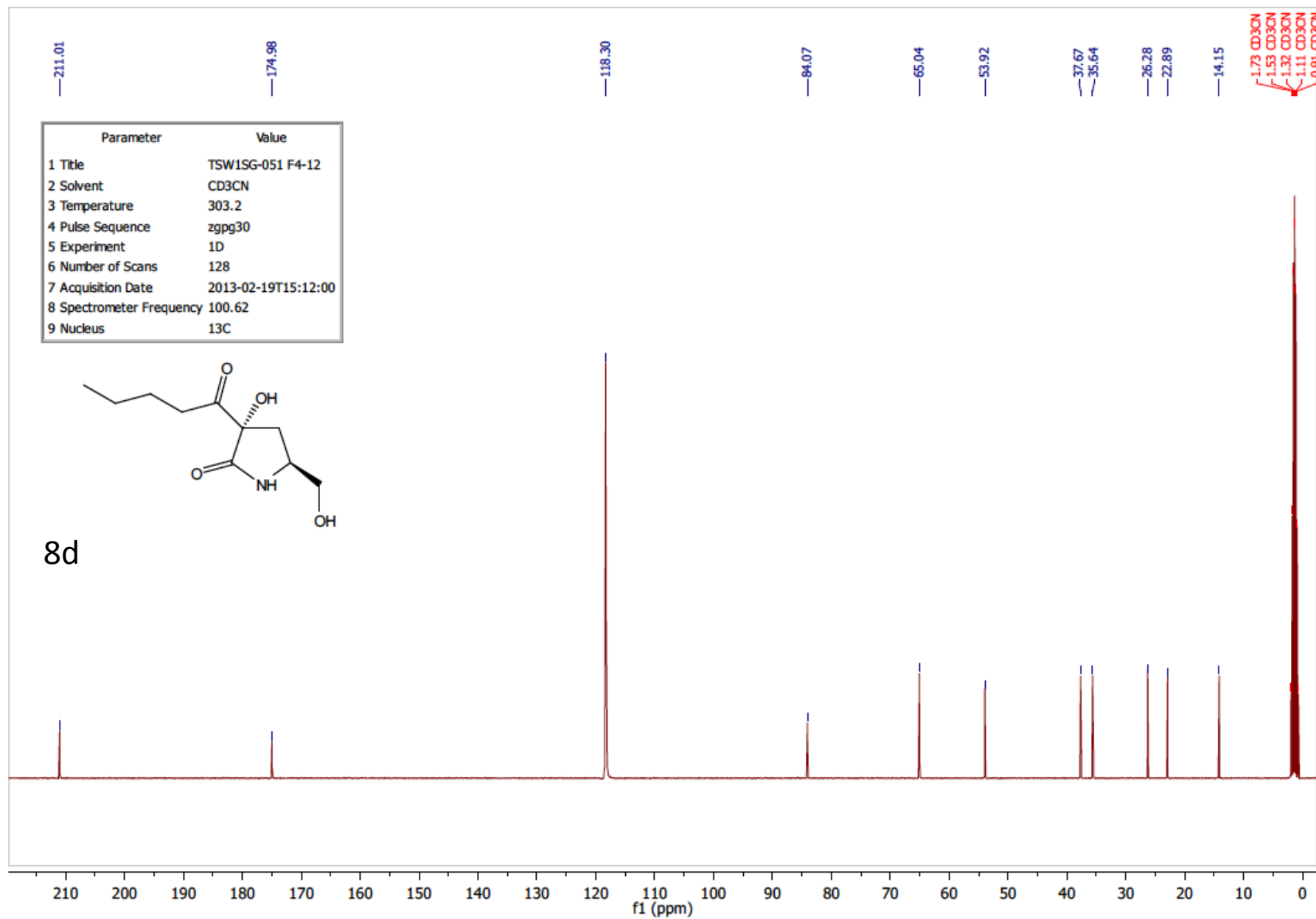


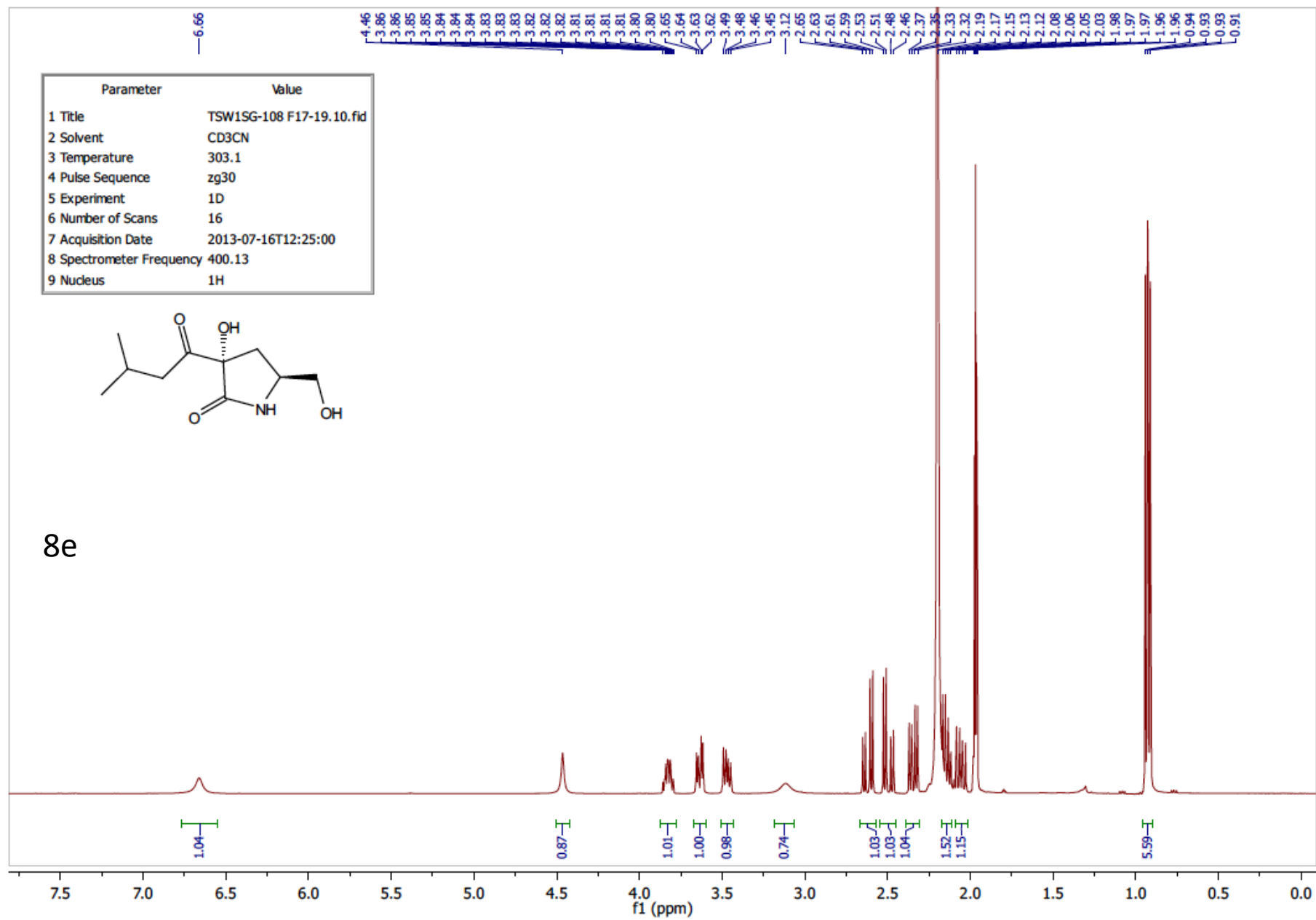


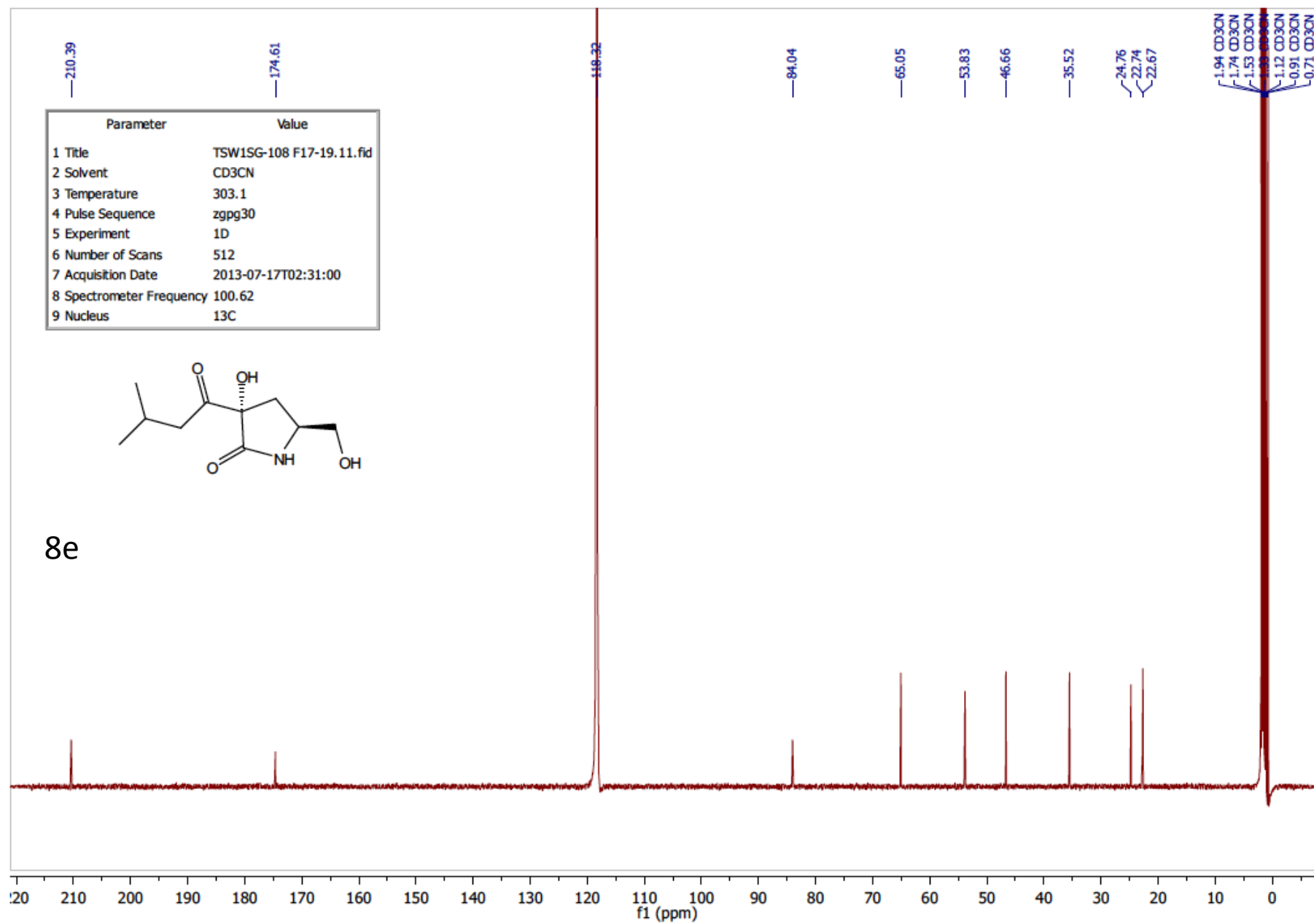


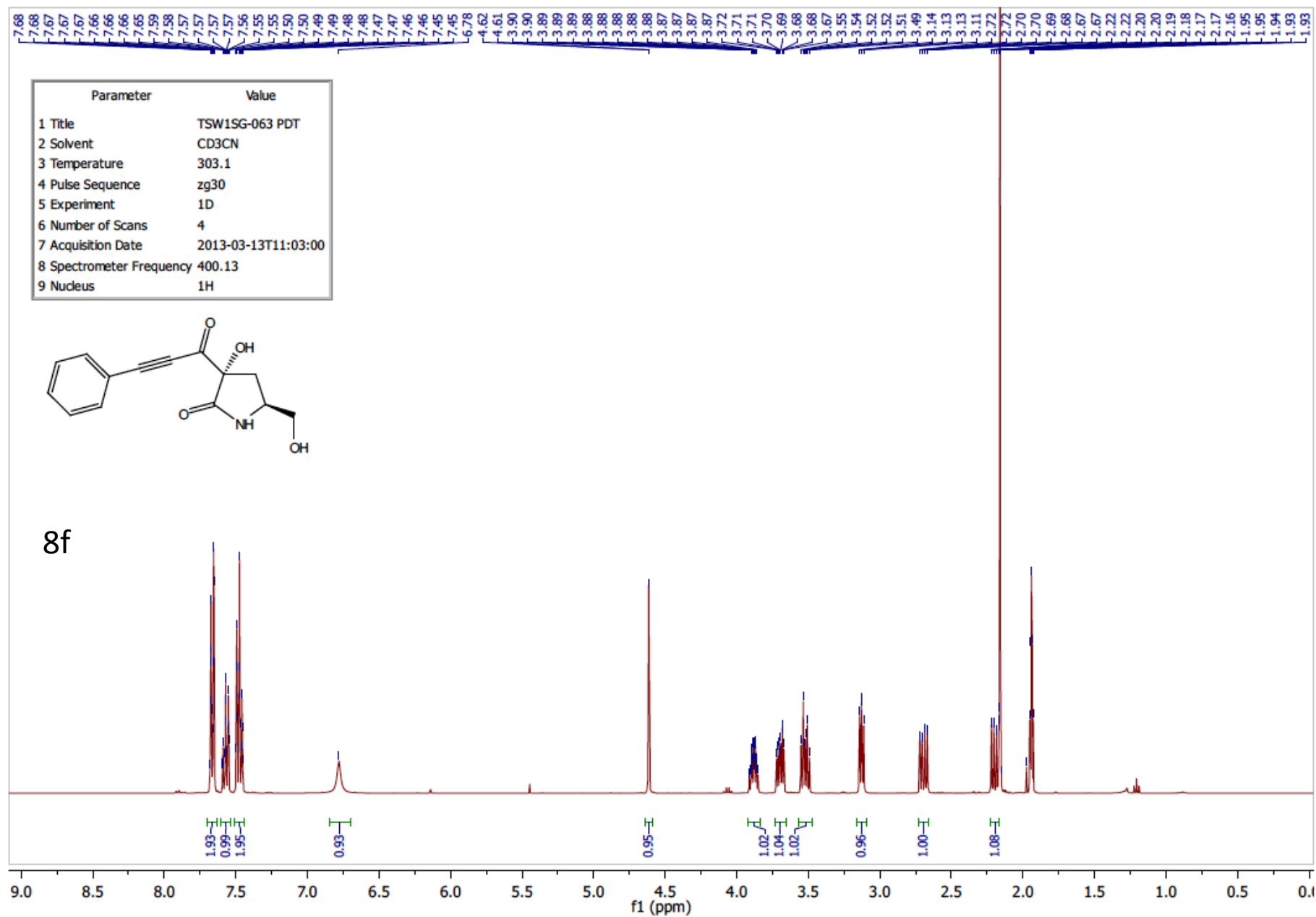


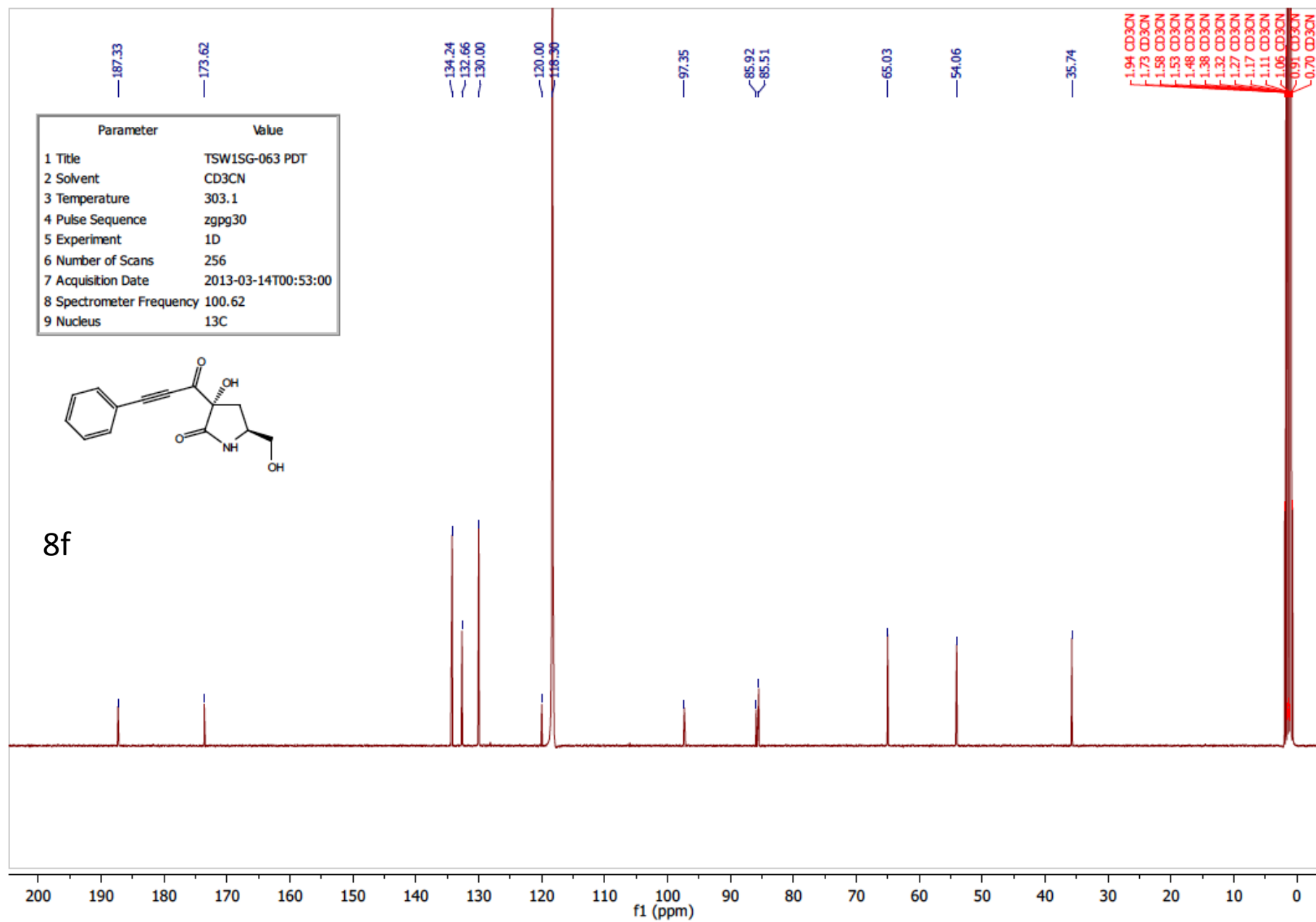


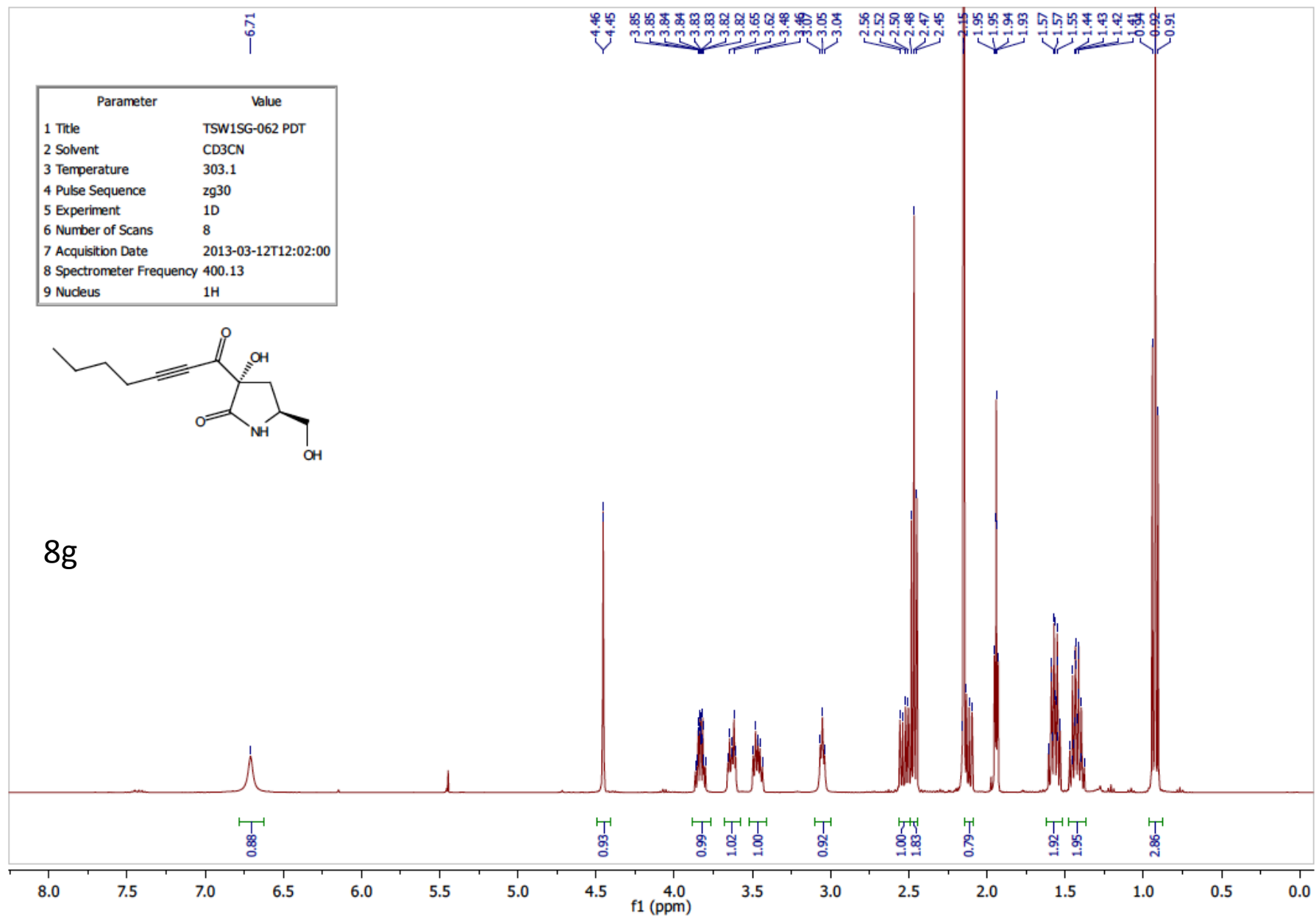


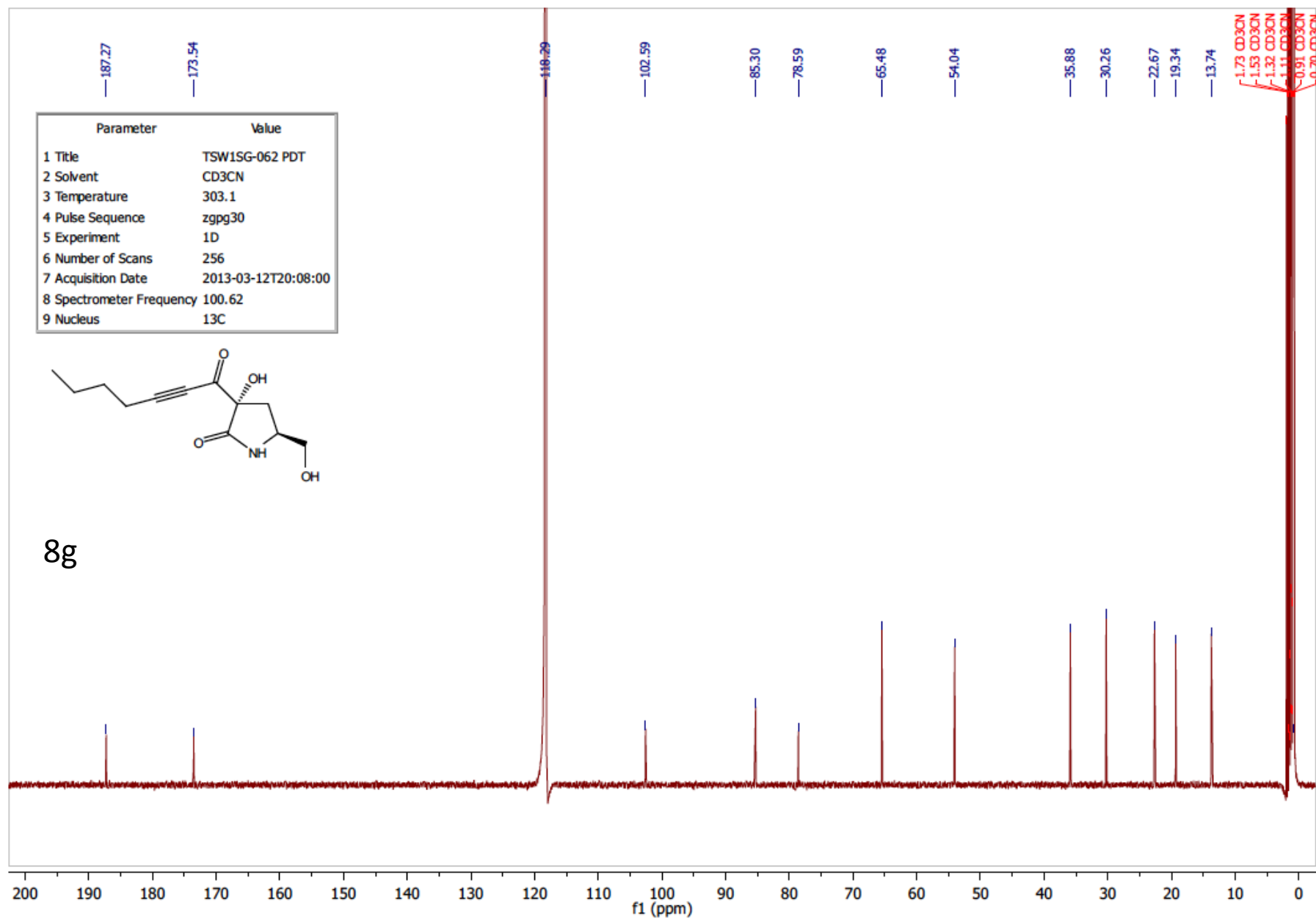


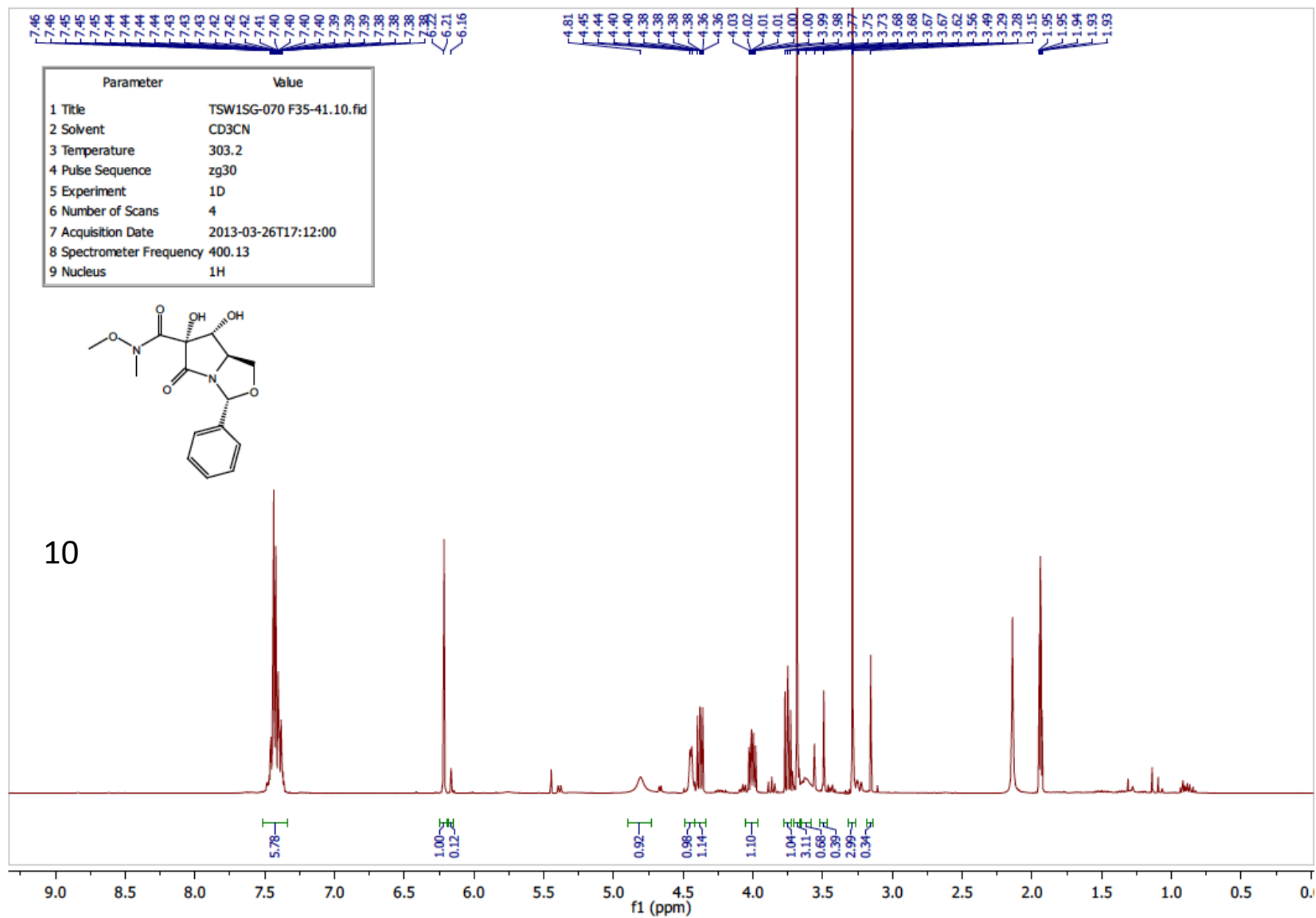


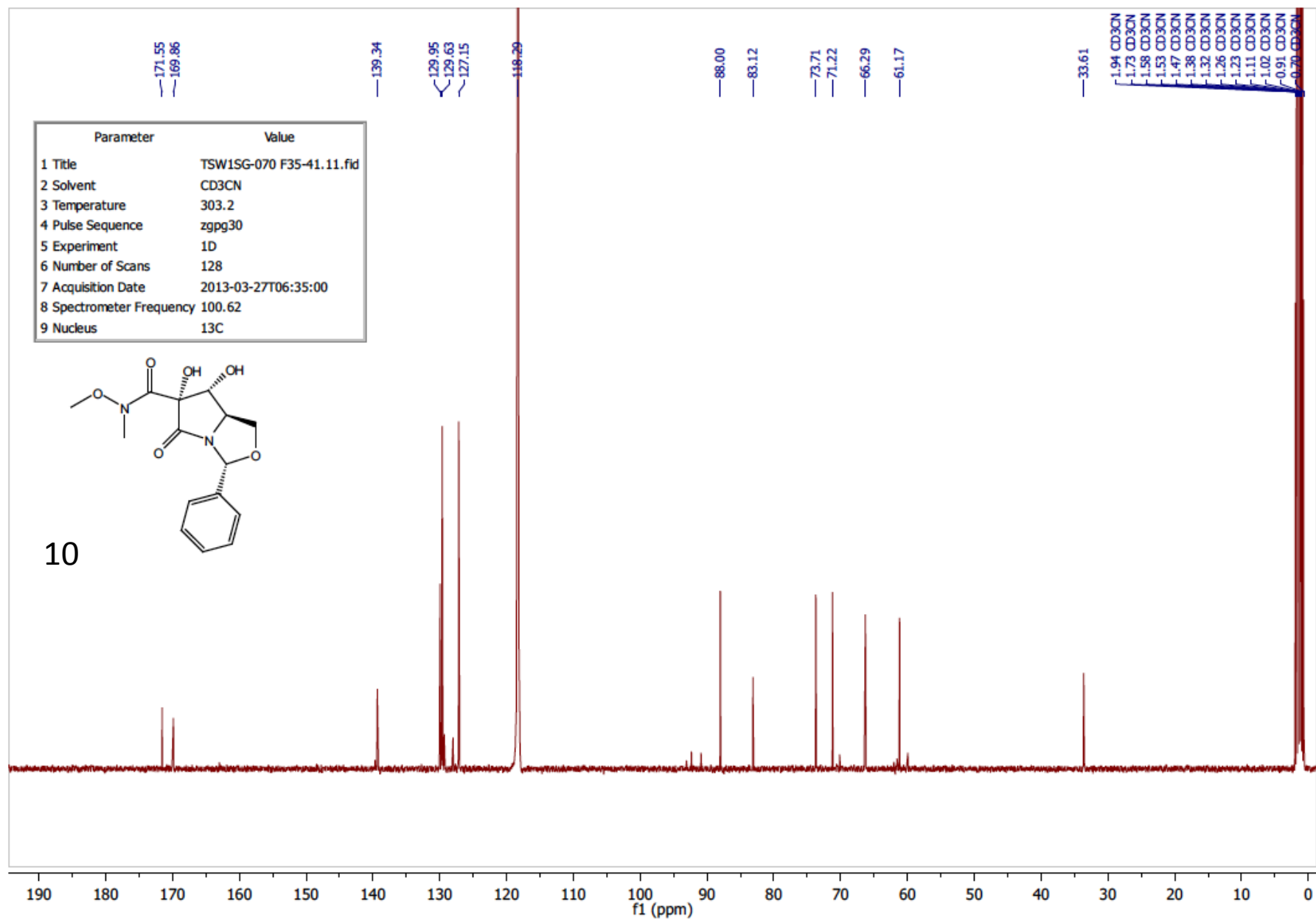


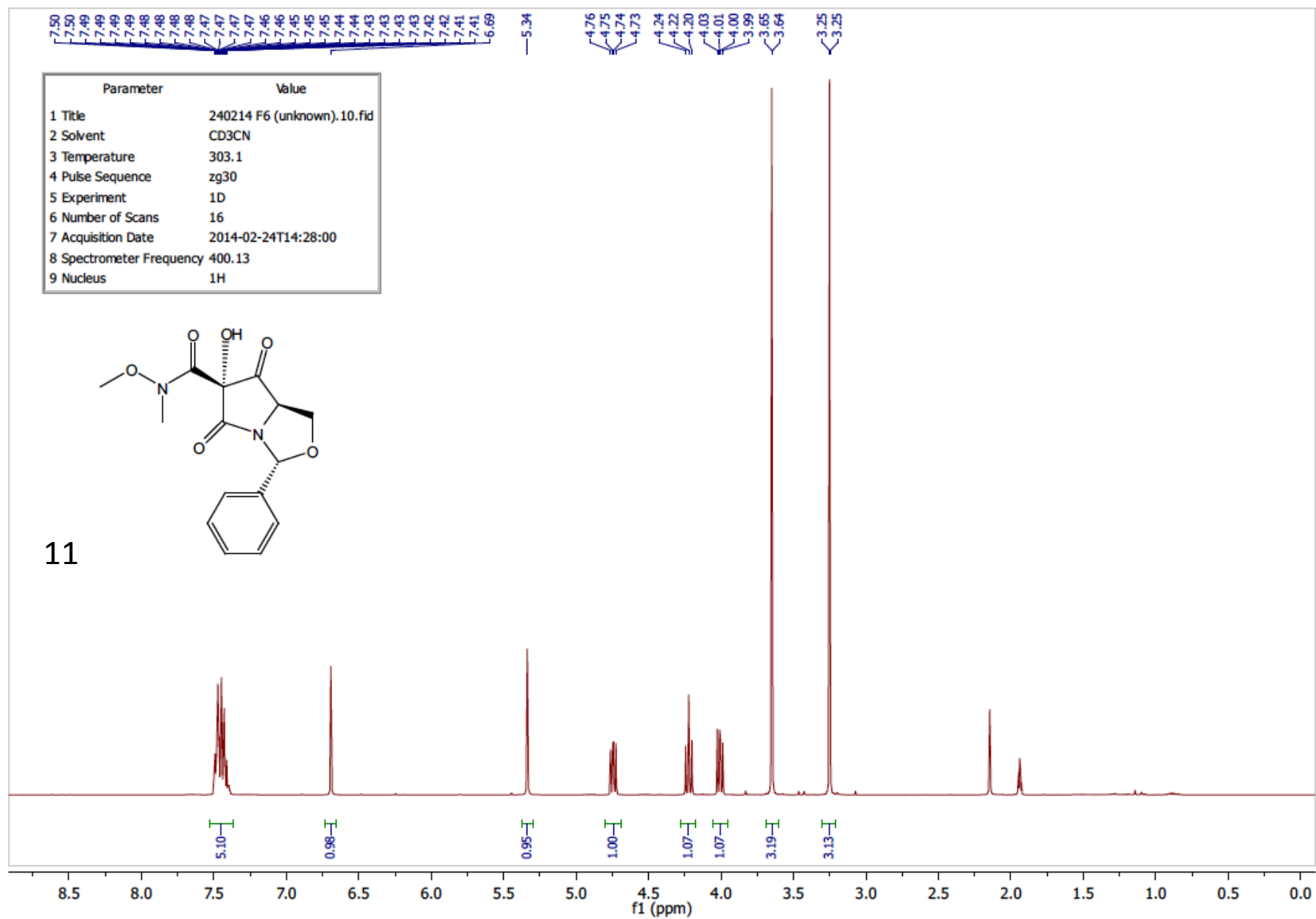


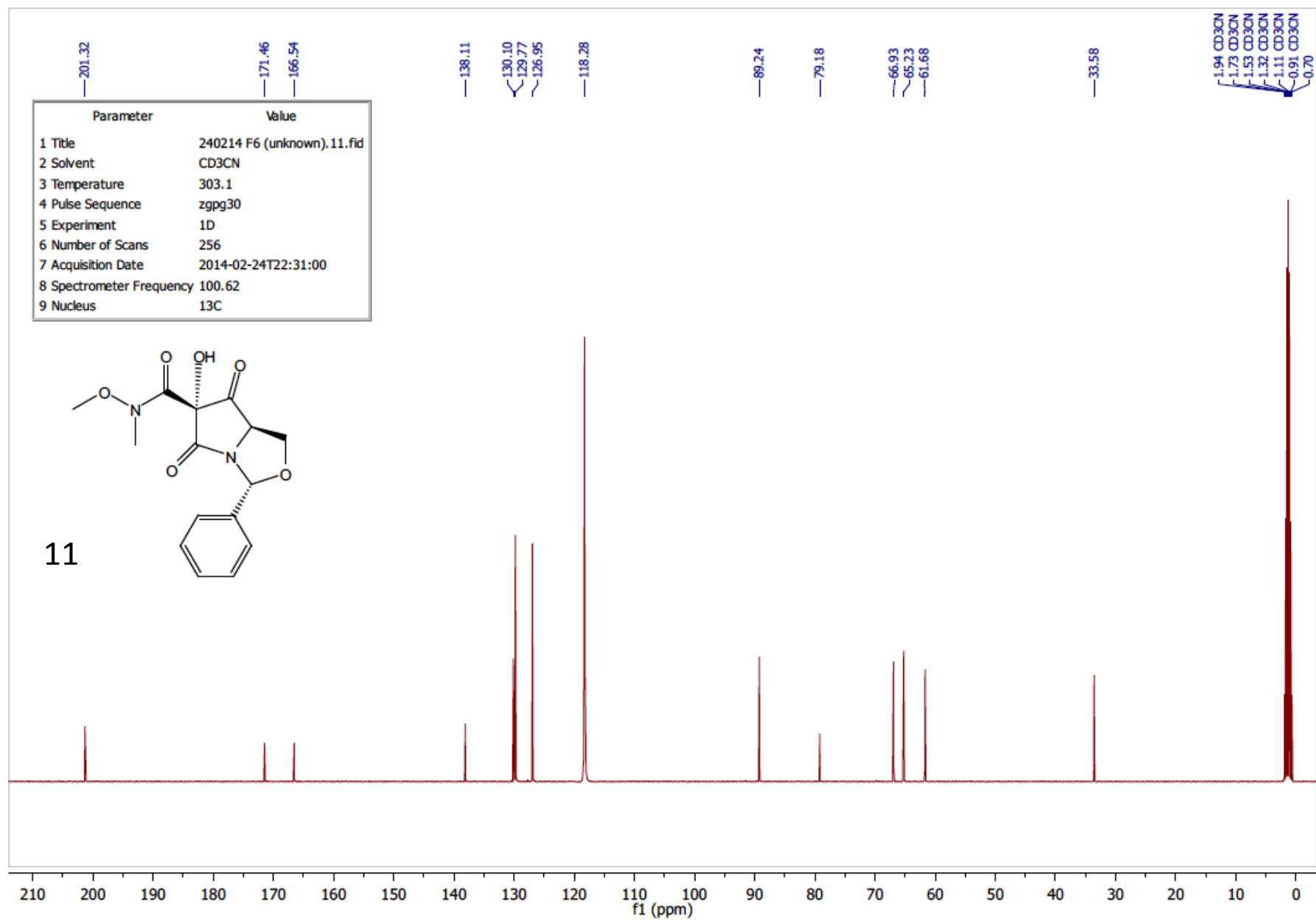


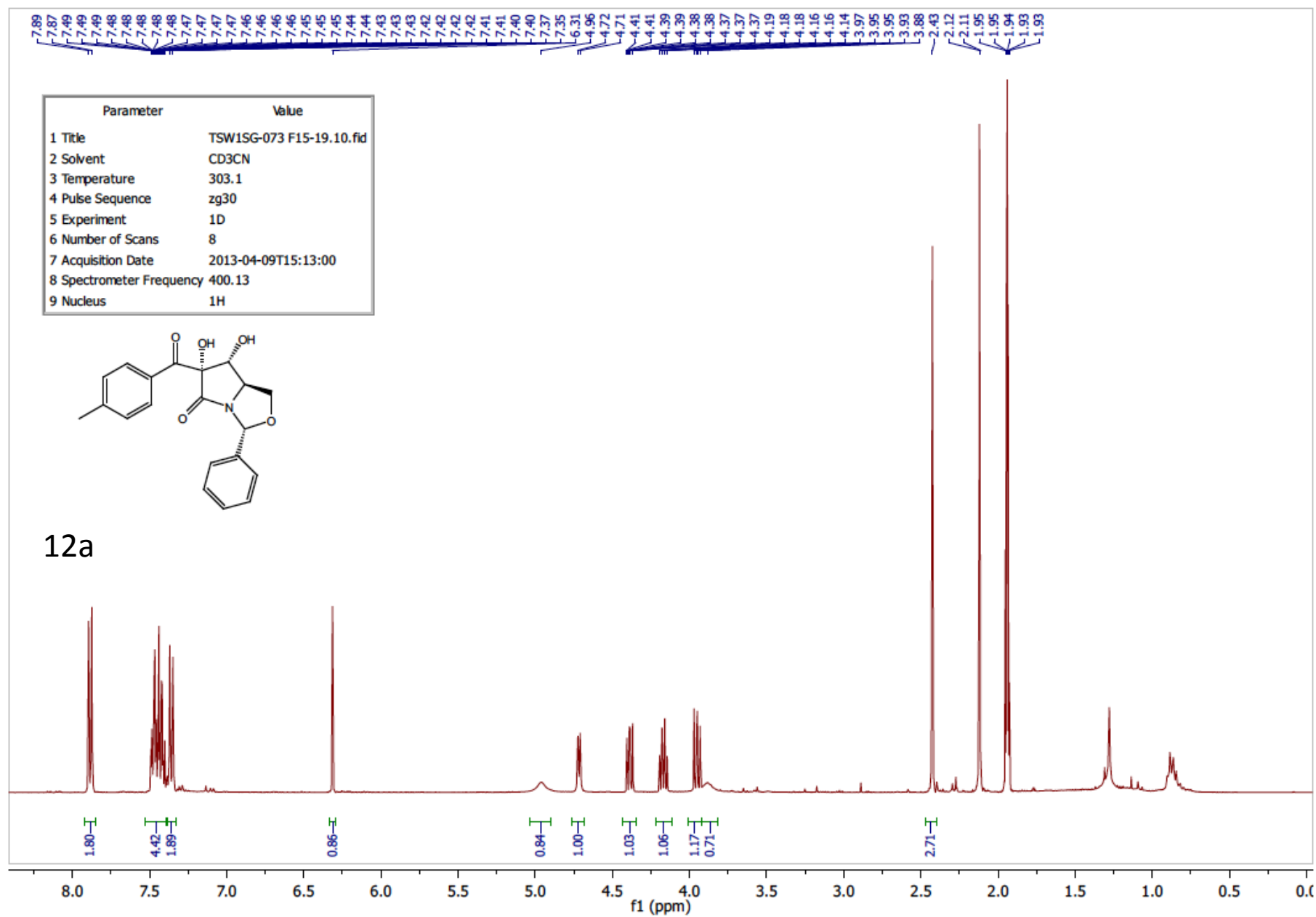


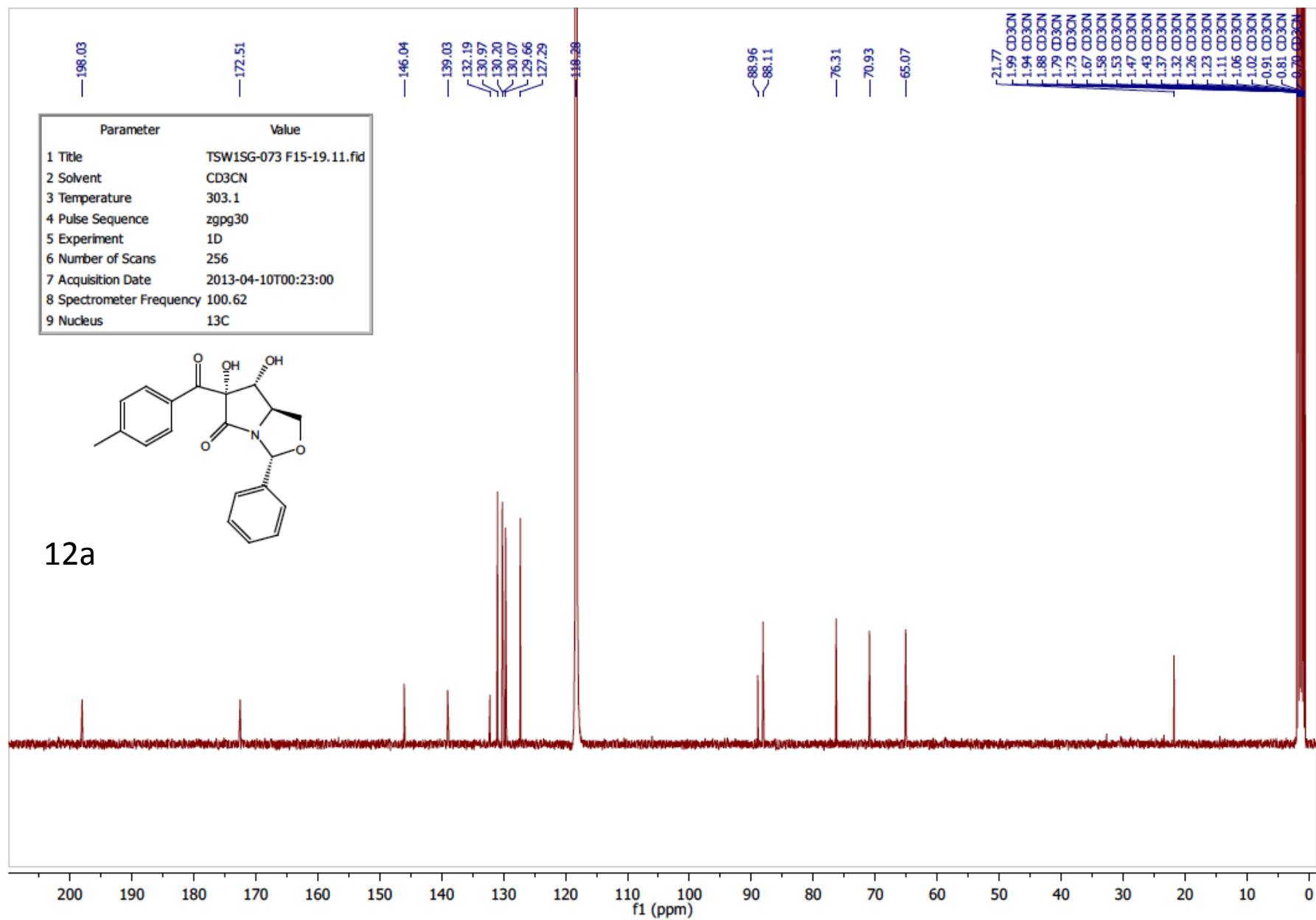


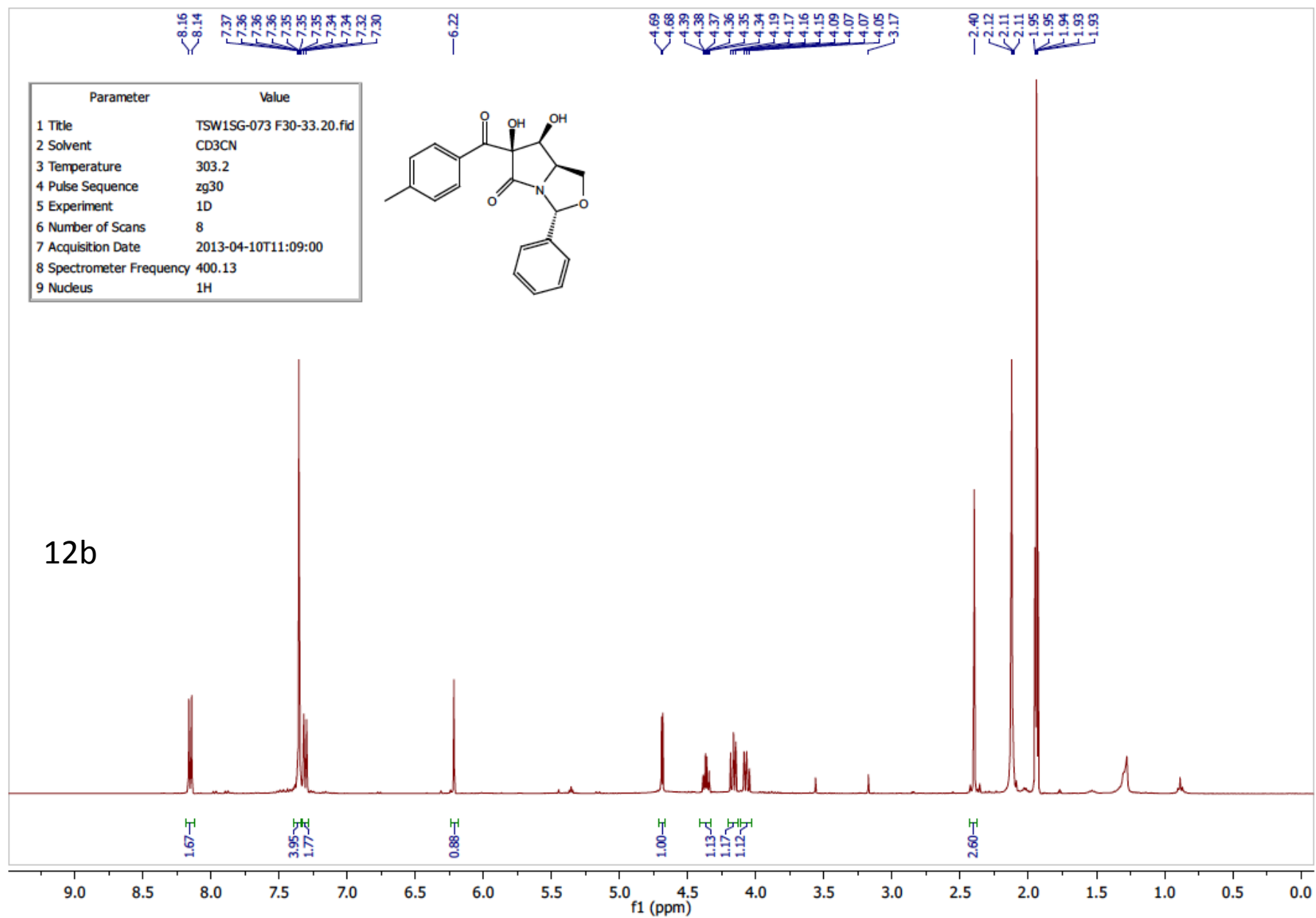


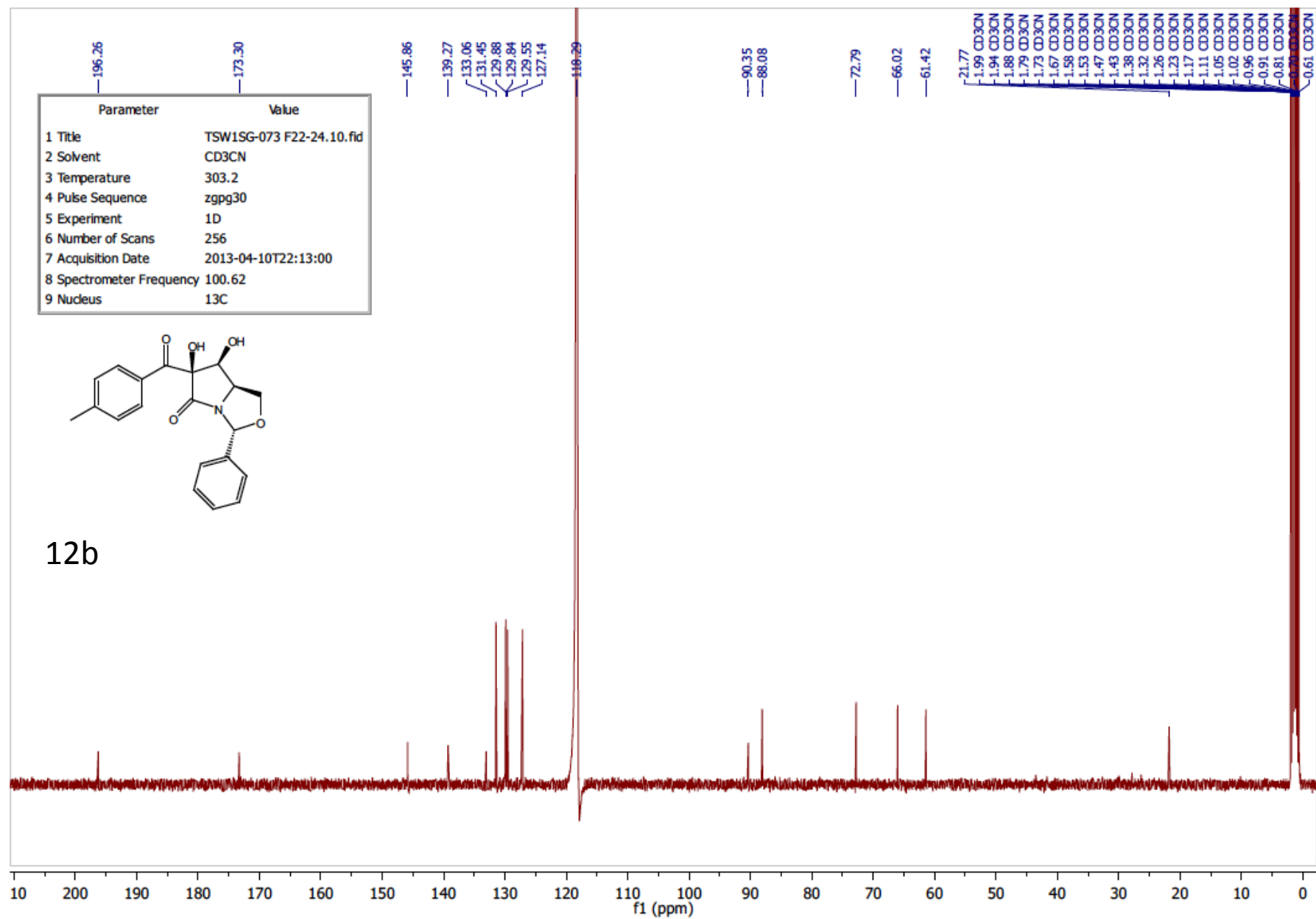


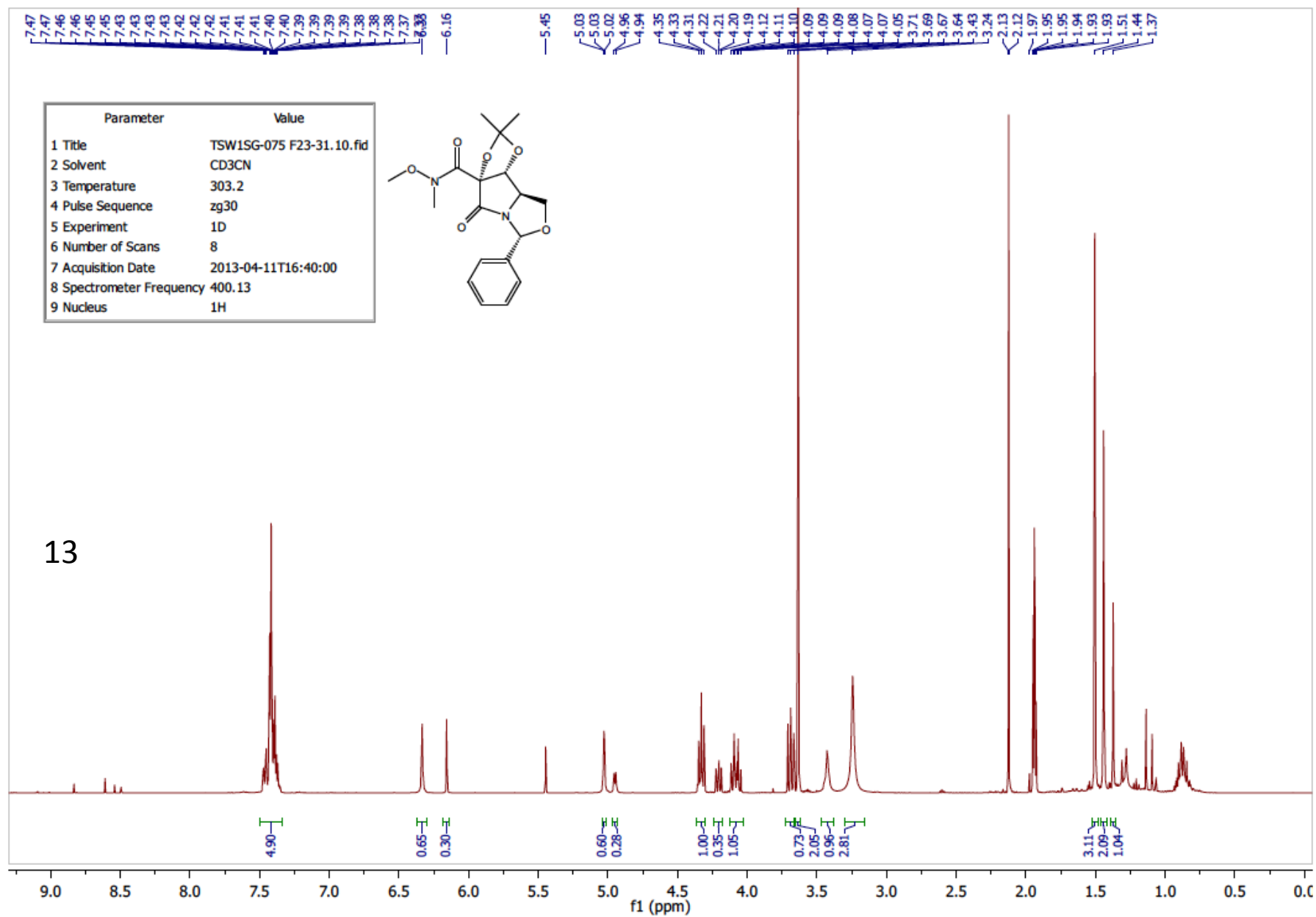


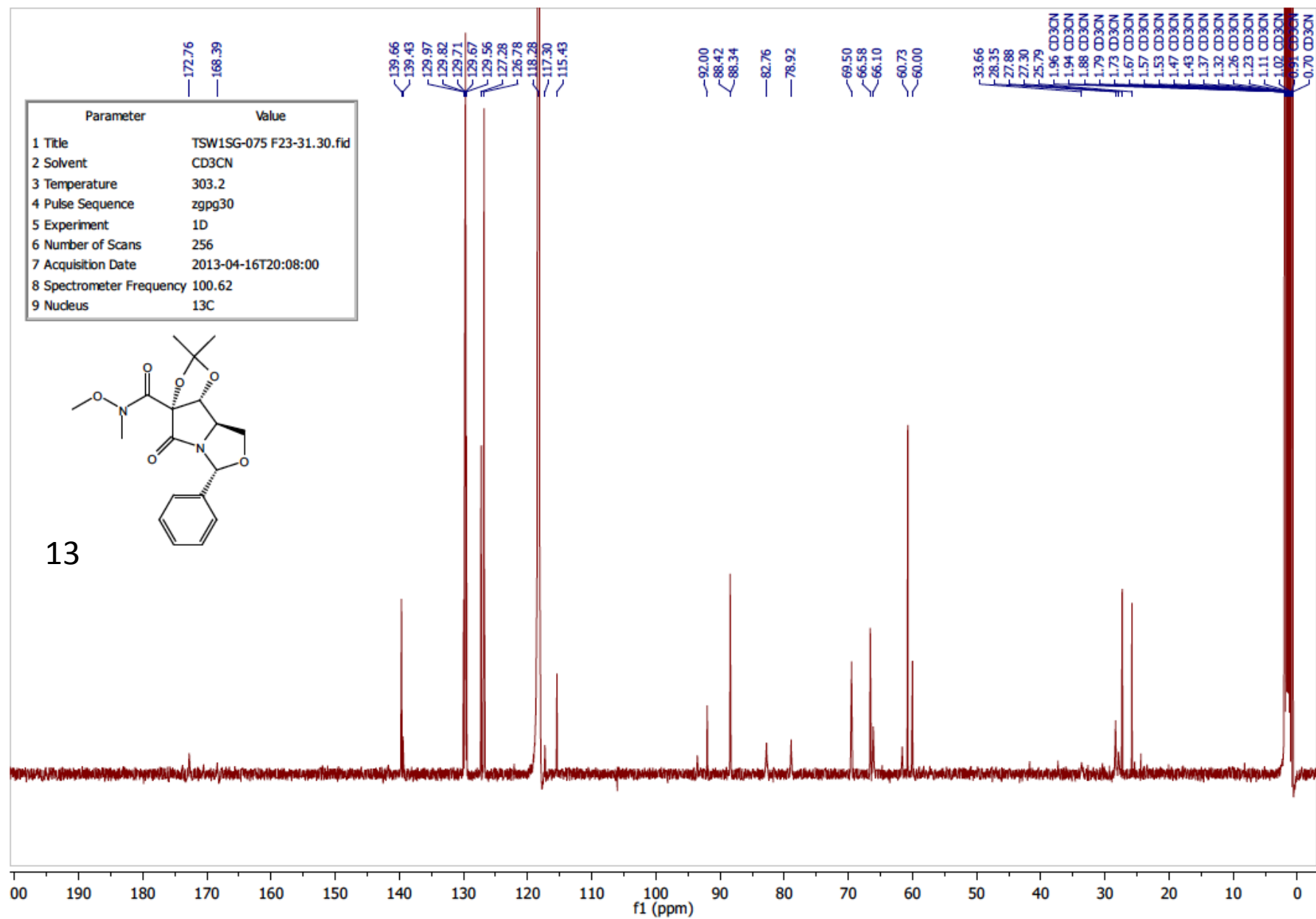


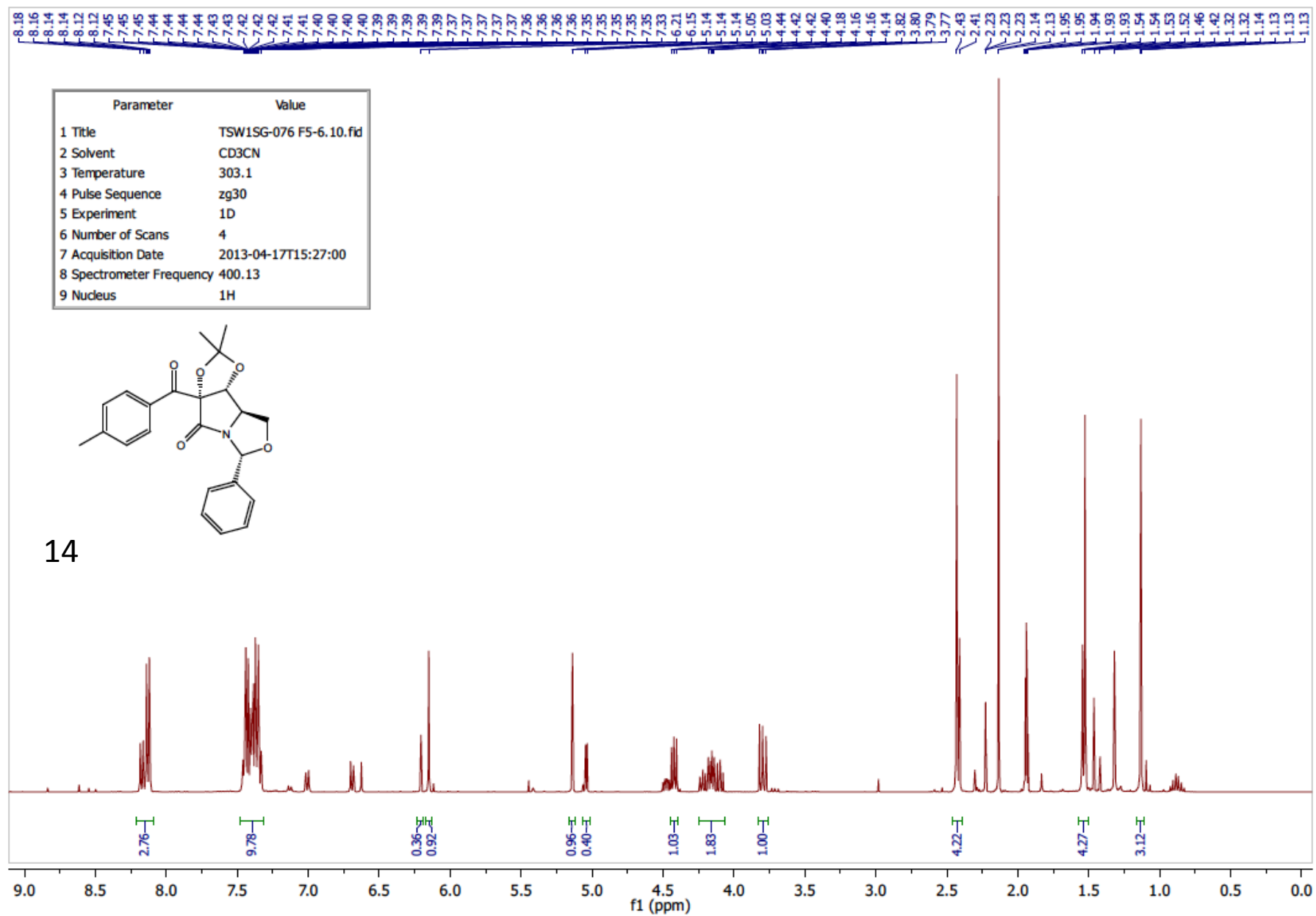


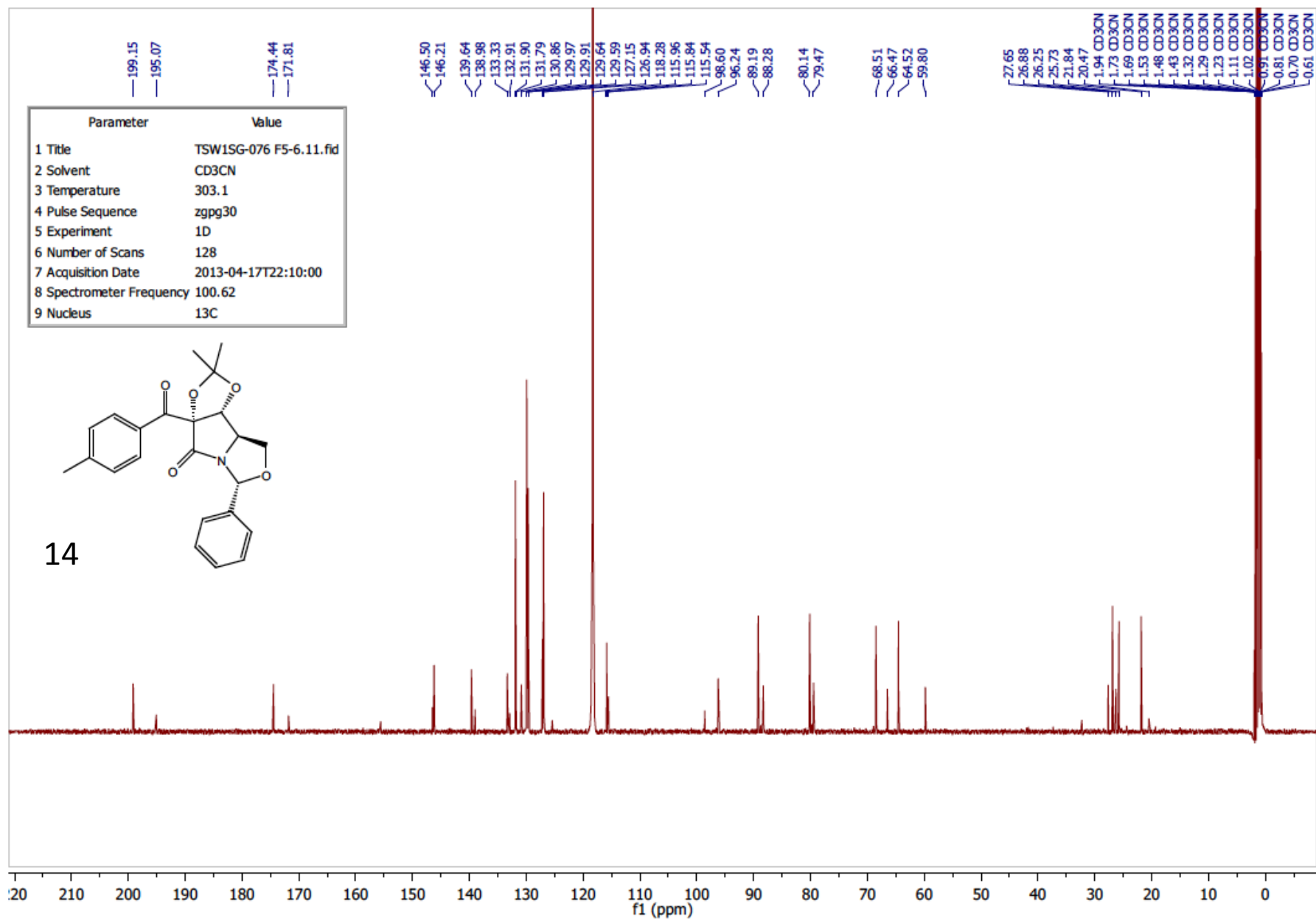


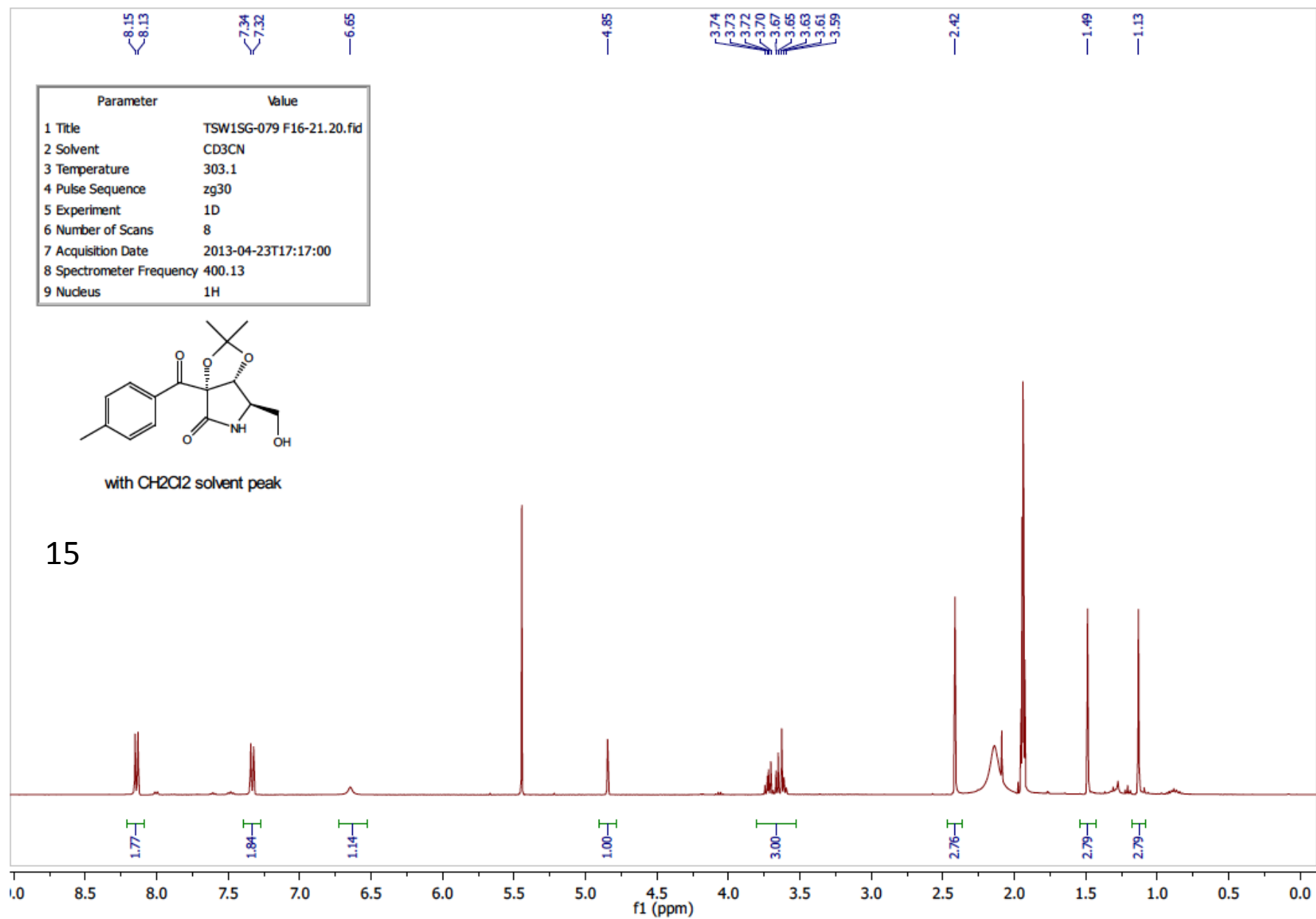


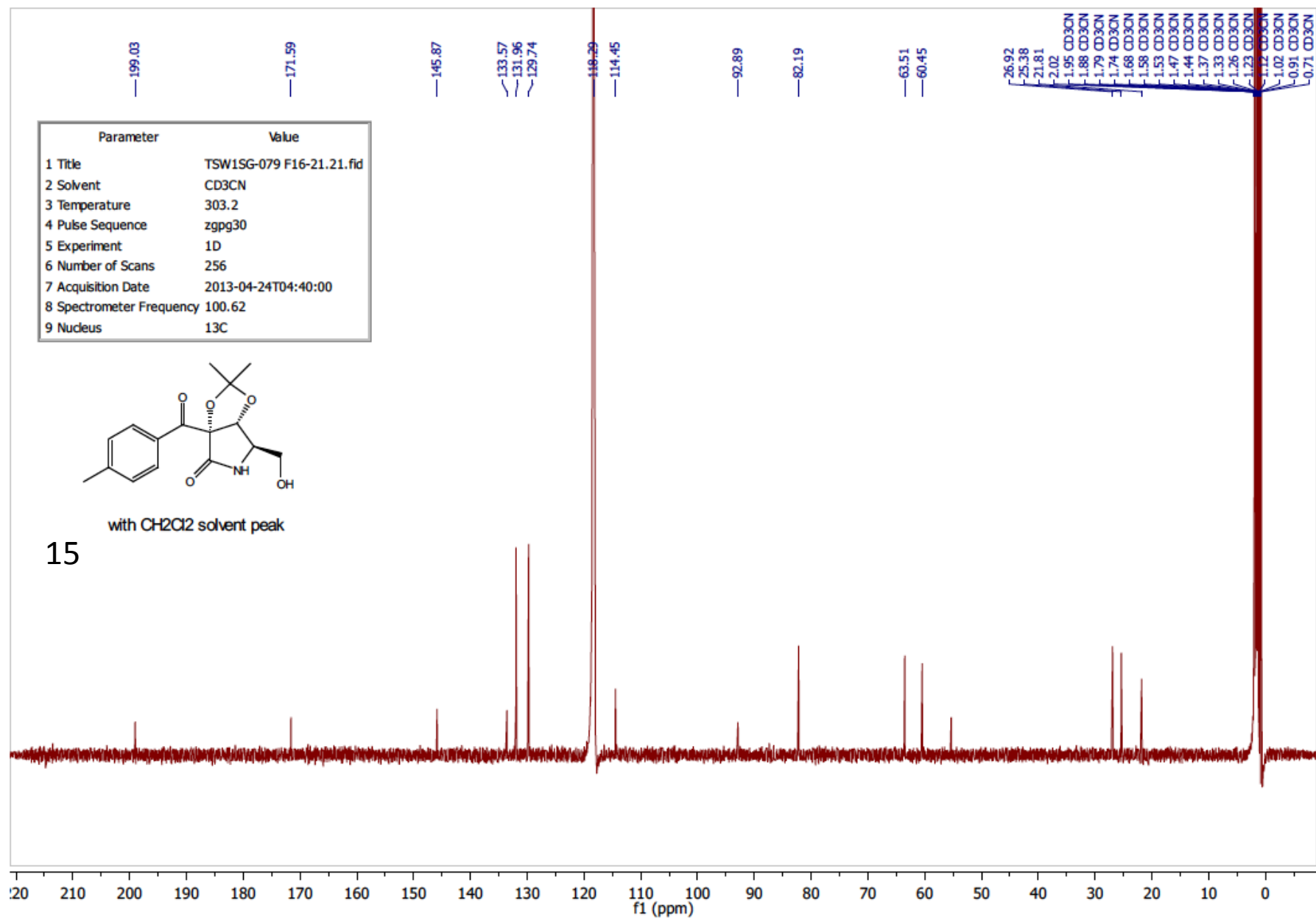


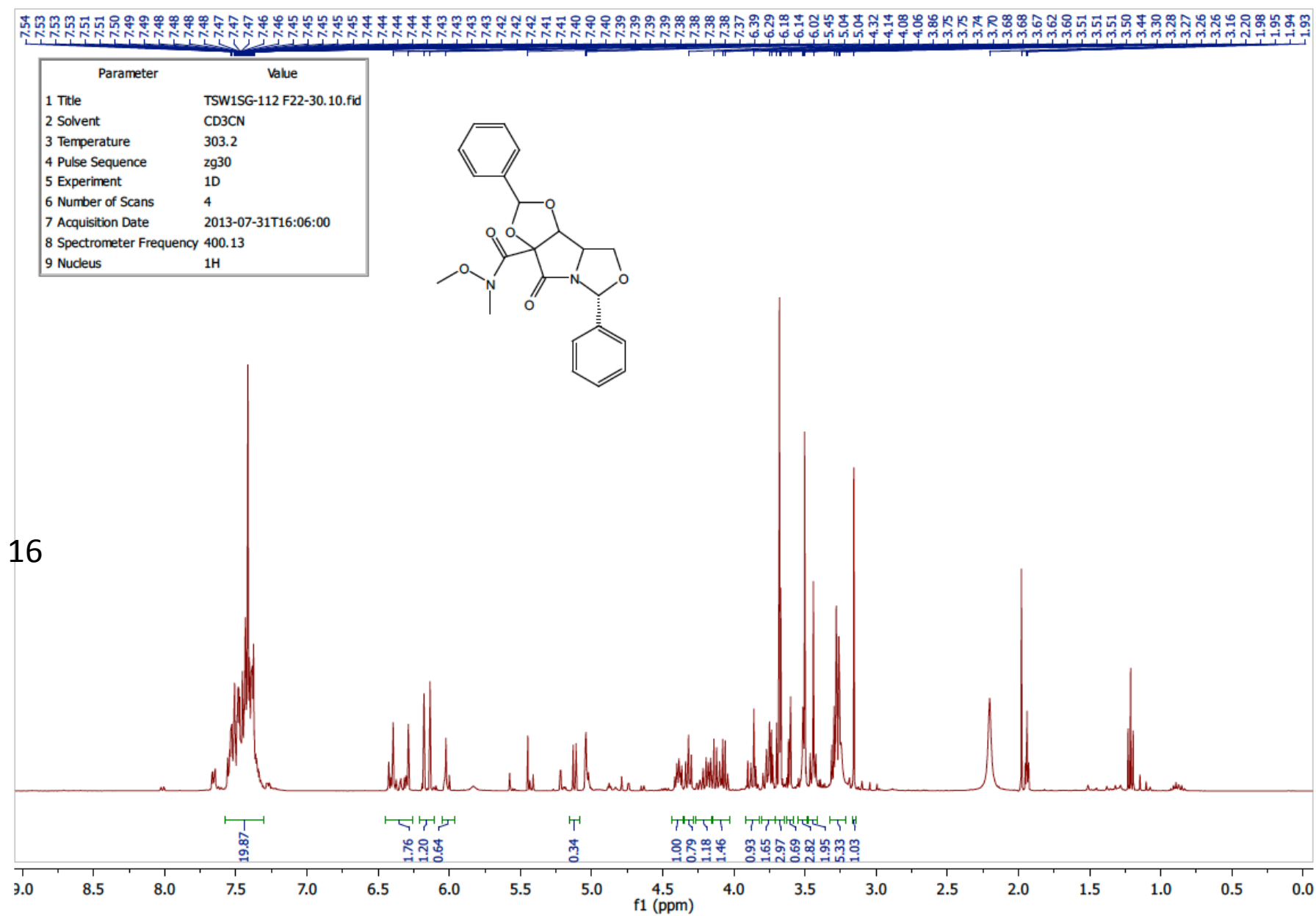




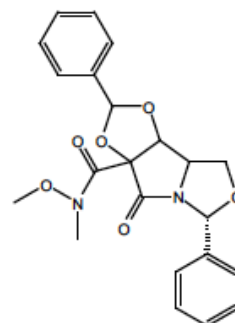




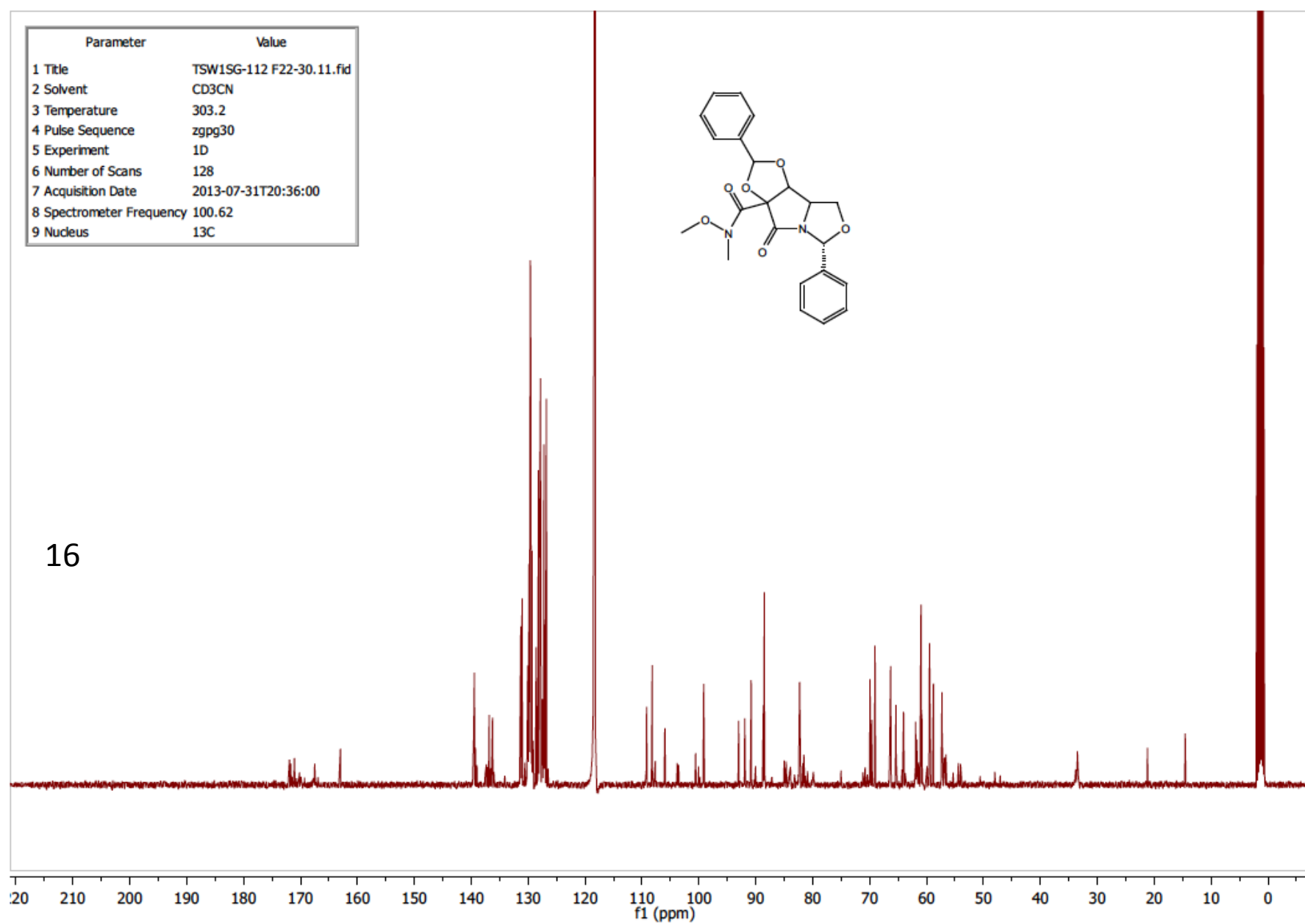


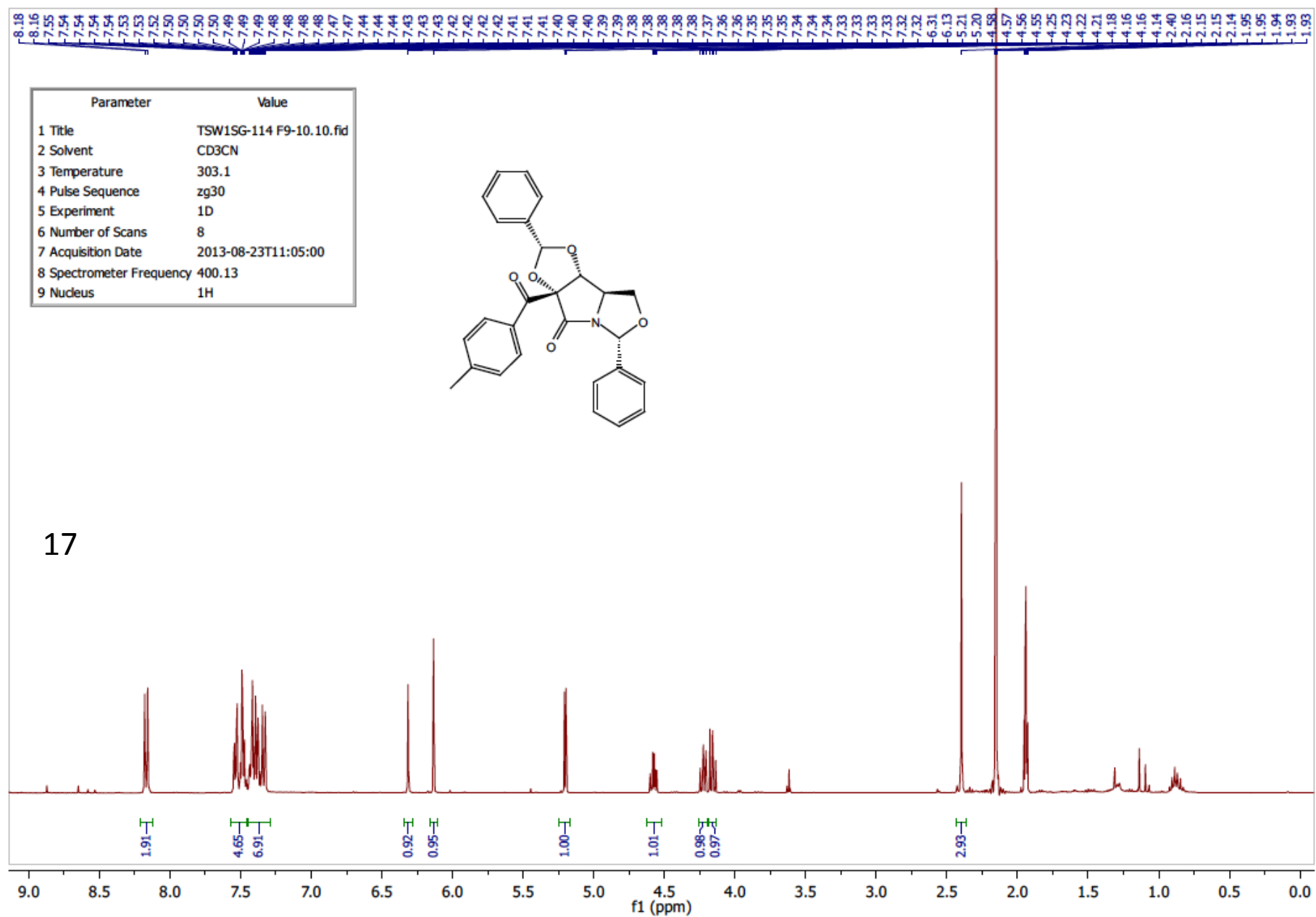


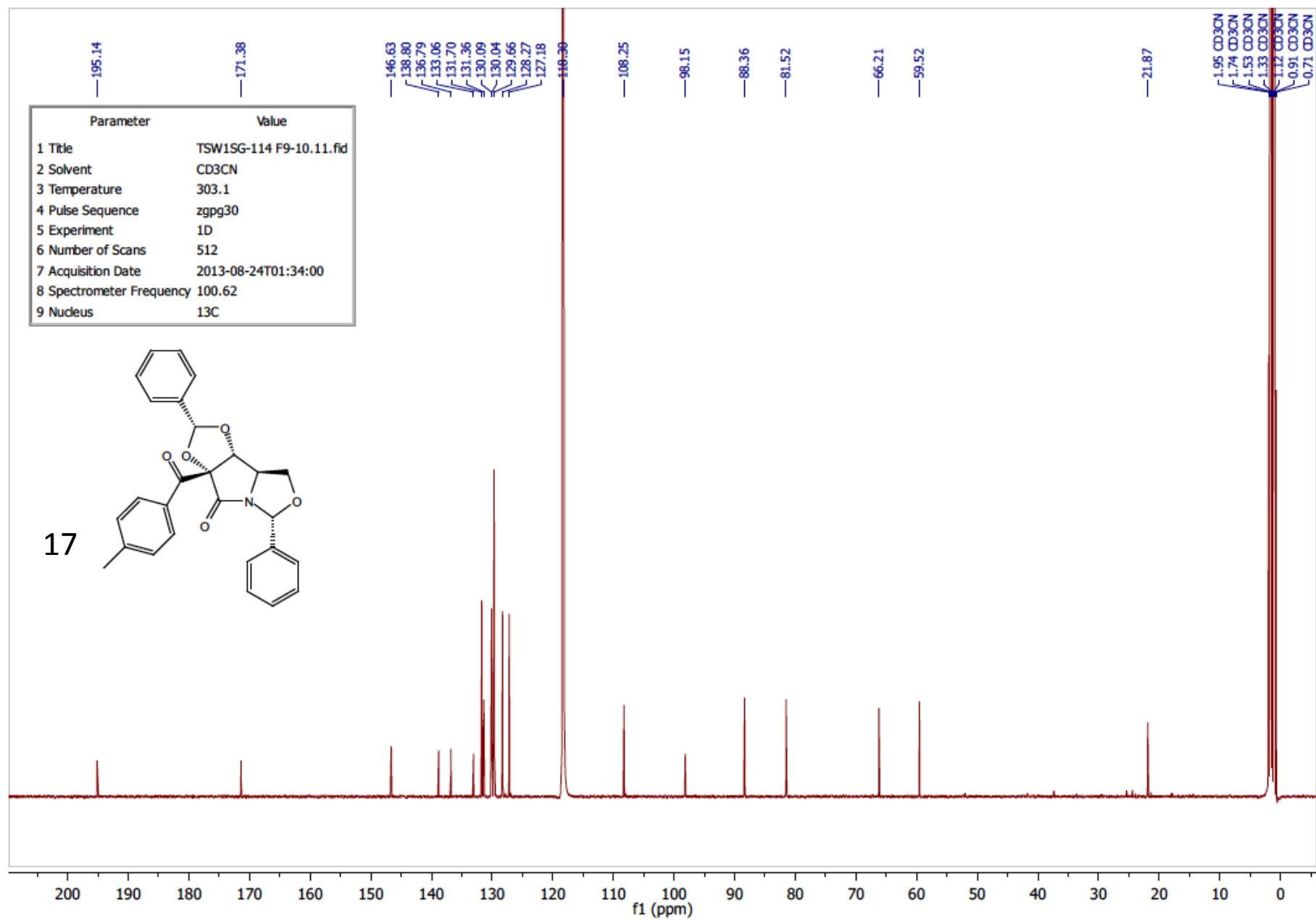
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| 3 Temperature            | 303.2                    |
| 4 Pulse Sequence         | zgpg30                   |
| 5 Experiment             | 1D                       |
| 6 Number of Scans        | 128                      |
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| 8 Spectrometer Frequency | 100.62                   |
| 9 Nucleus                | <sup>13</sup> C          |



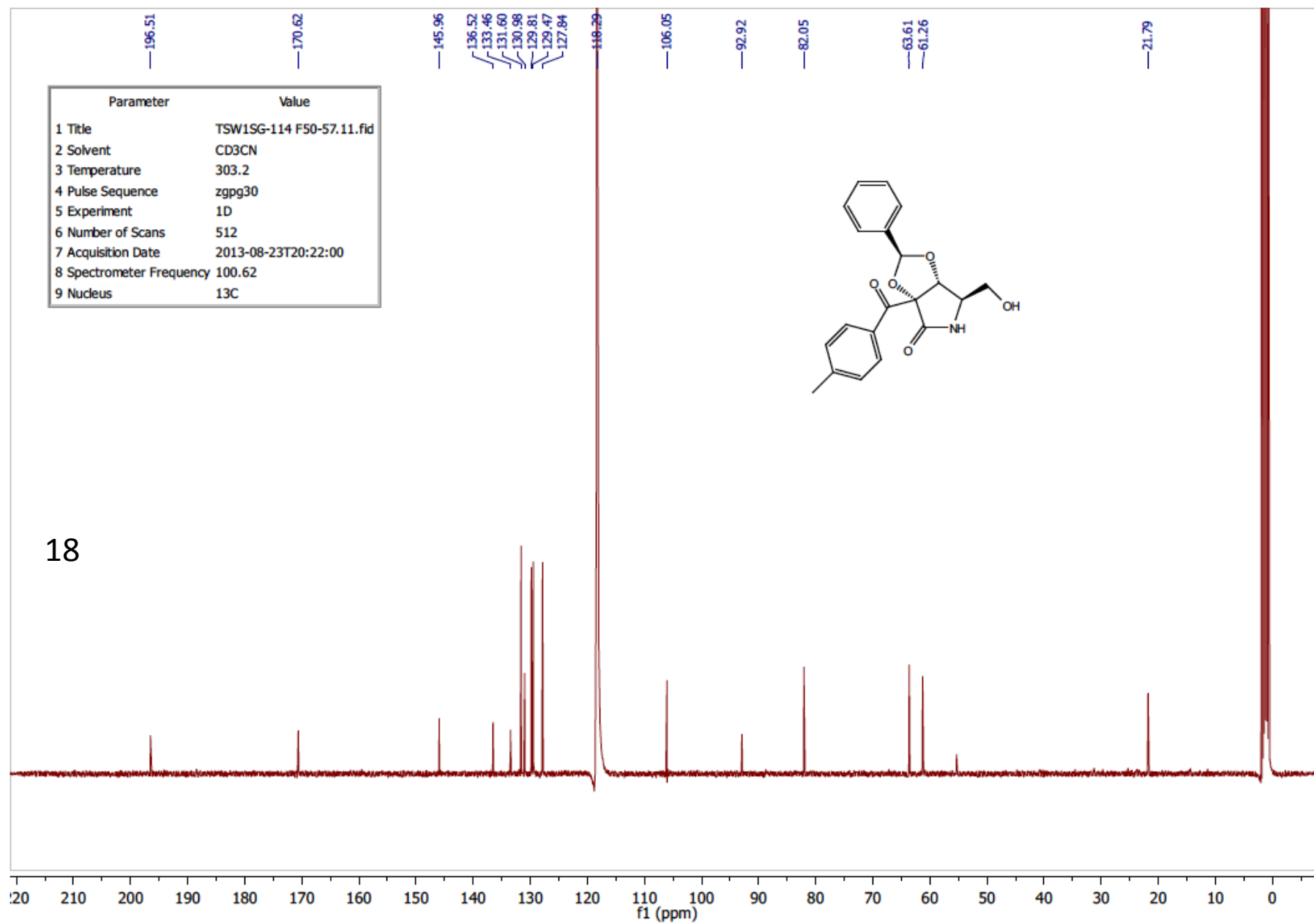
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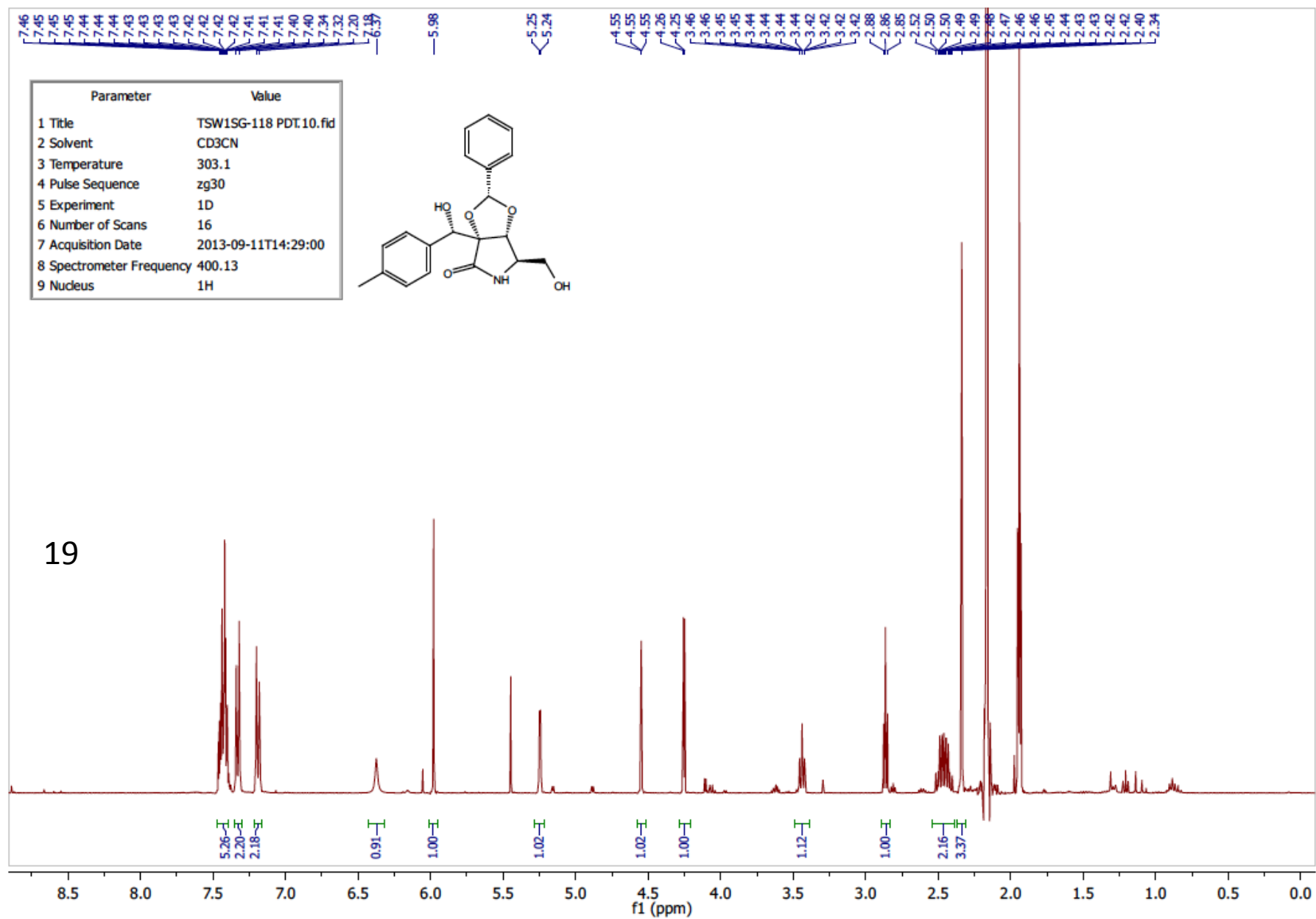


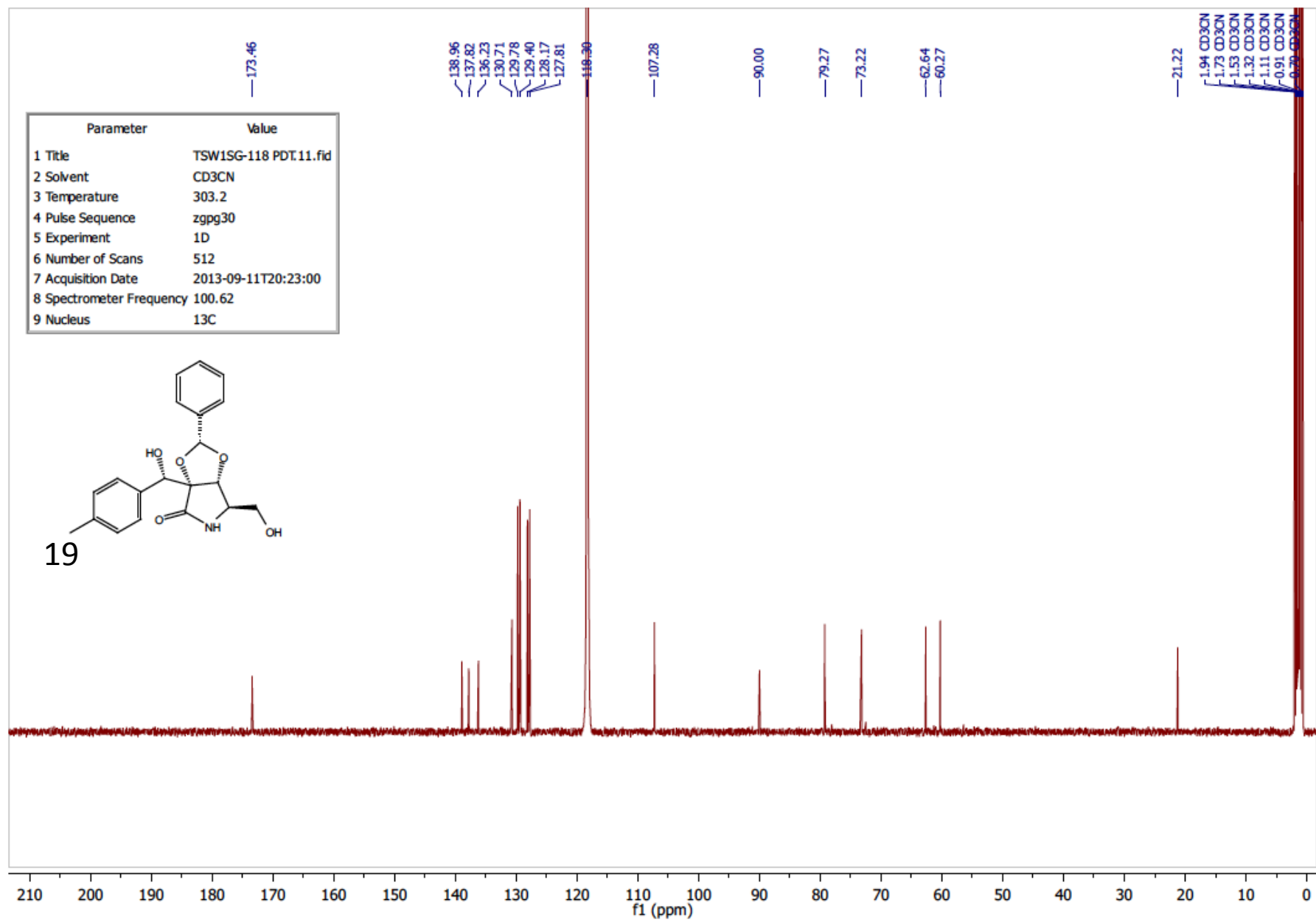


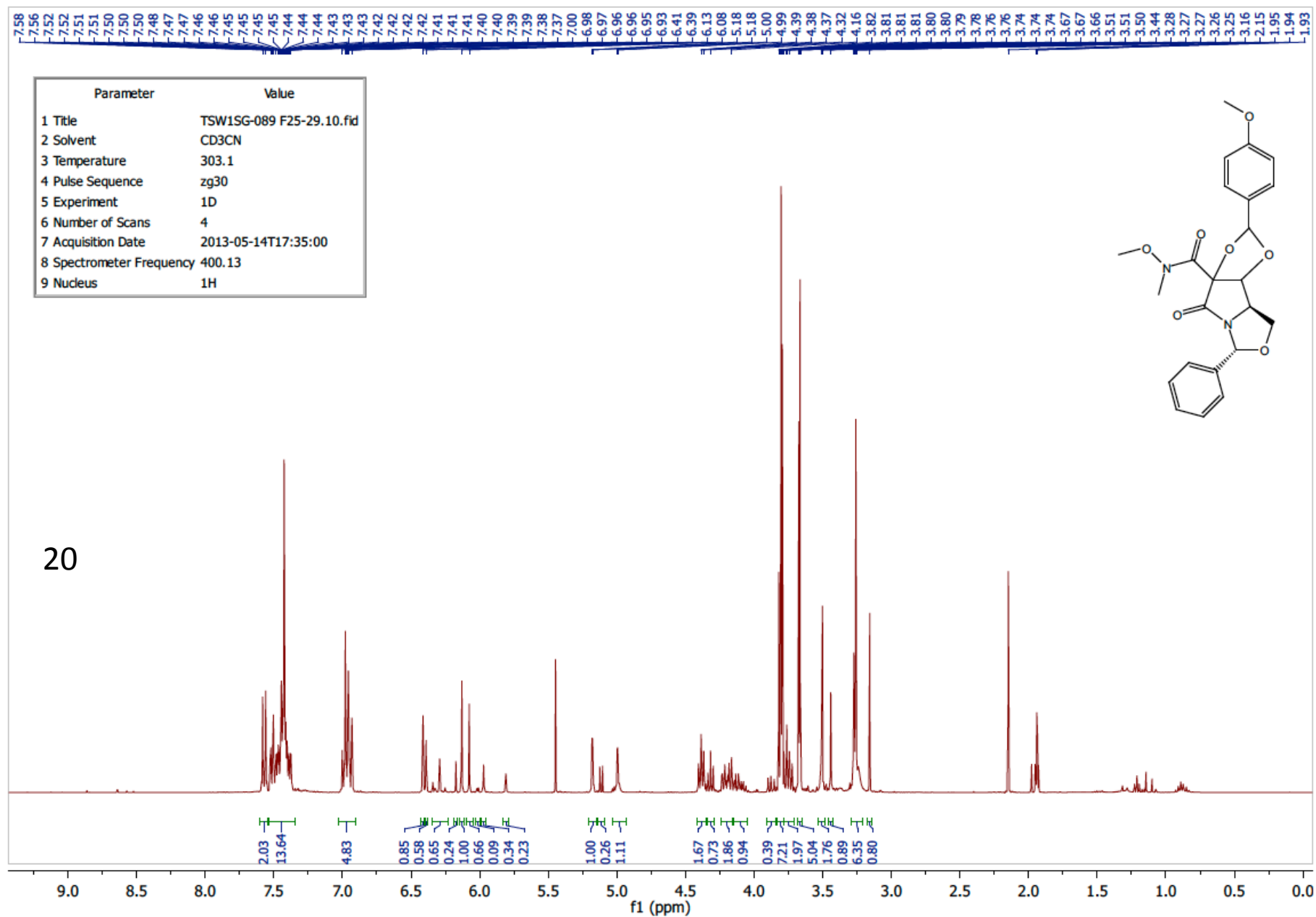


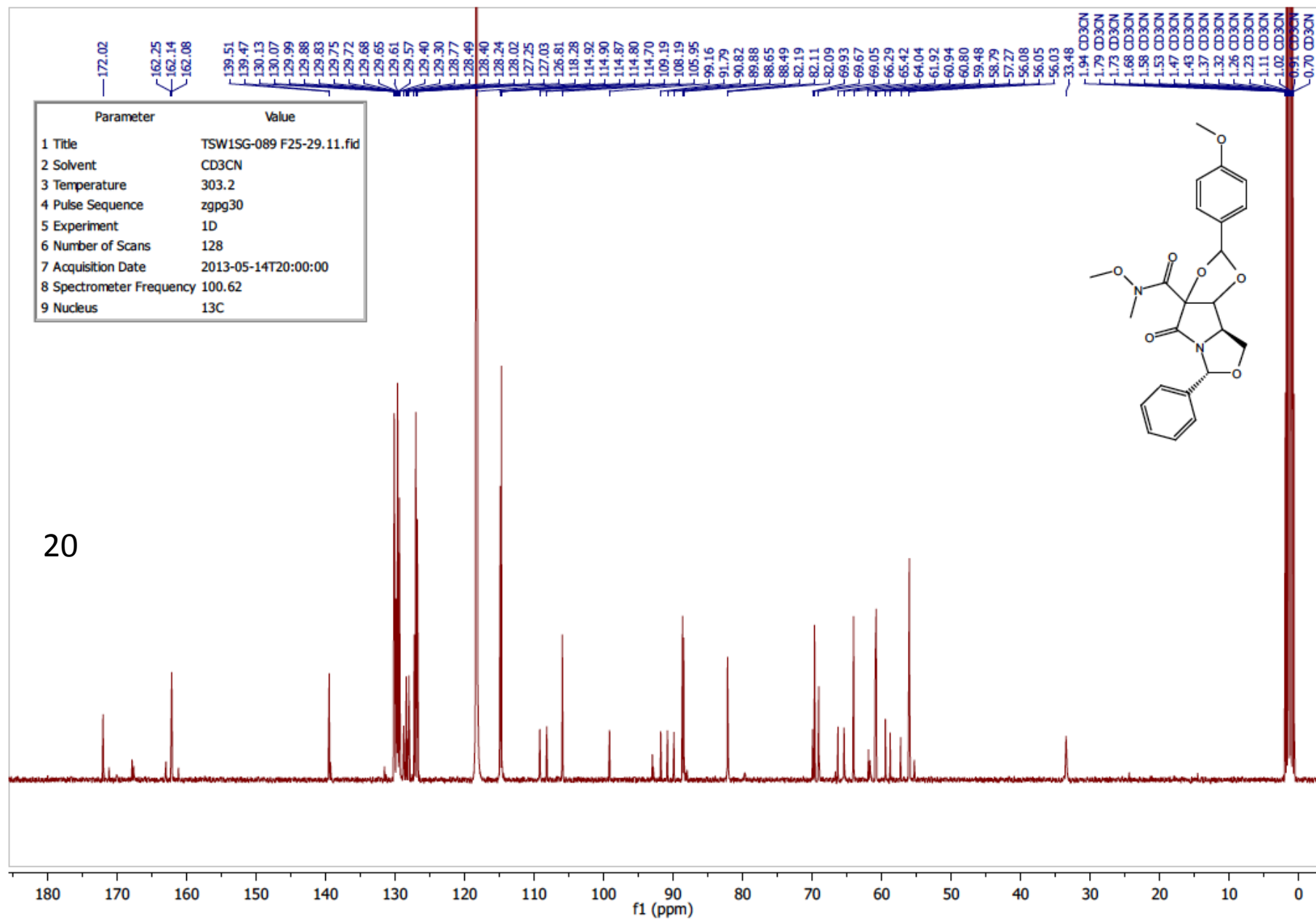


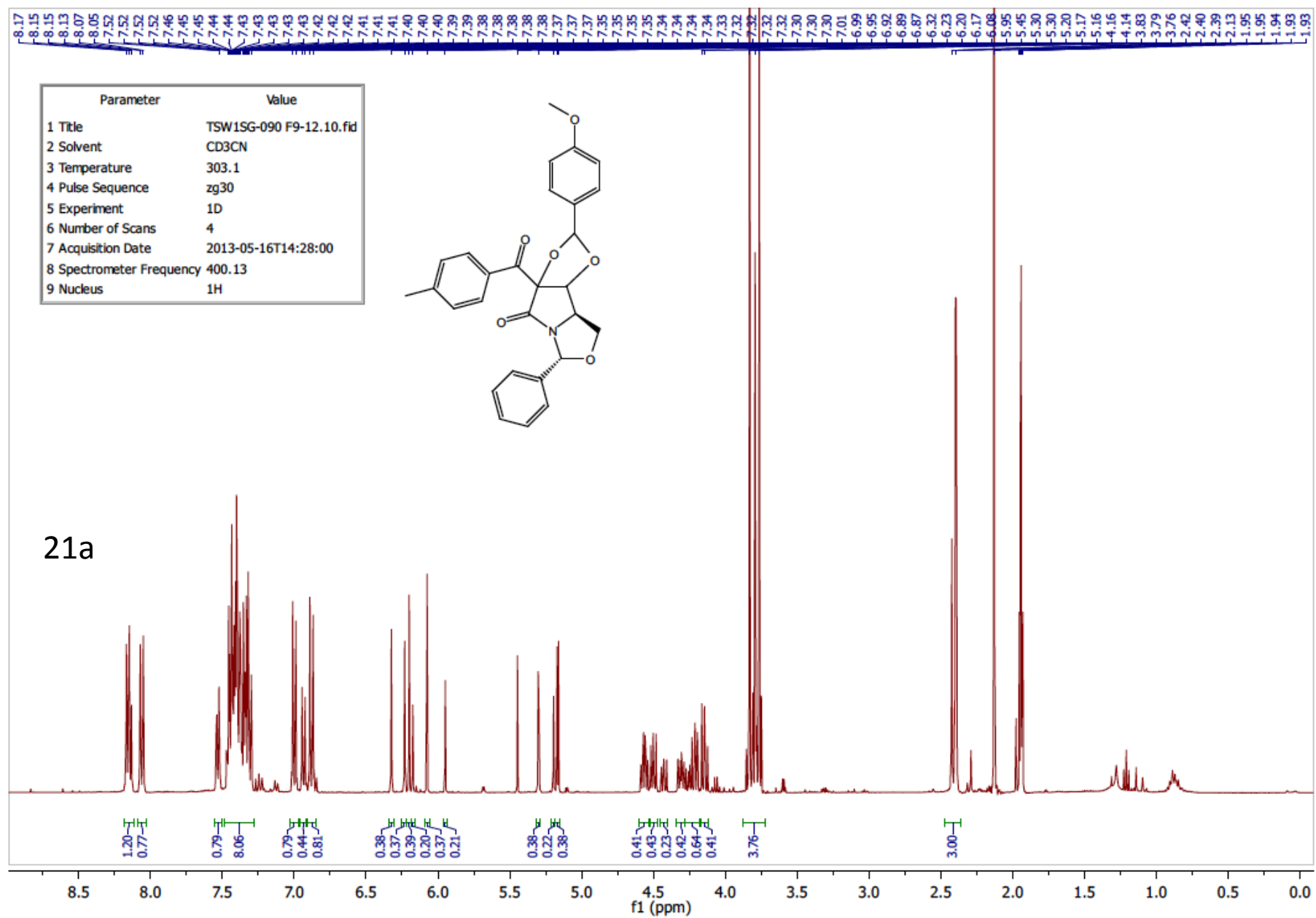


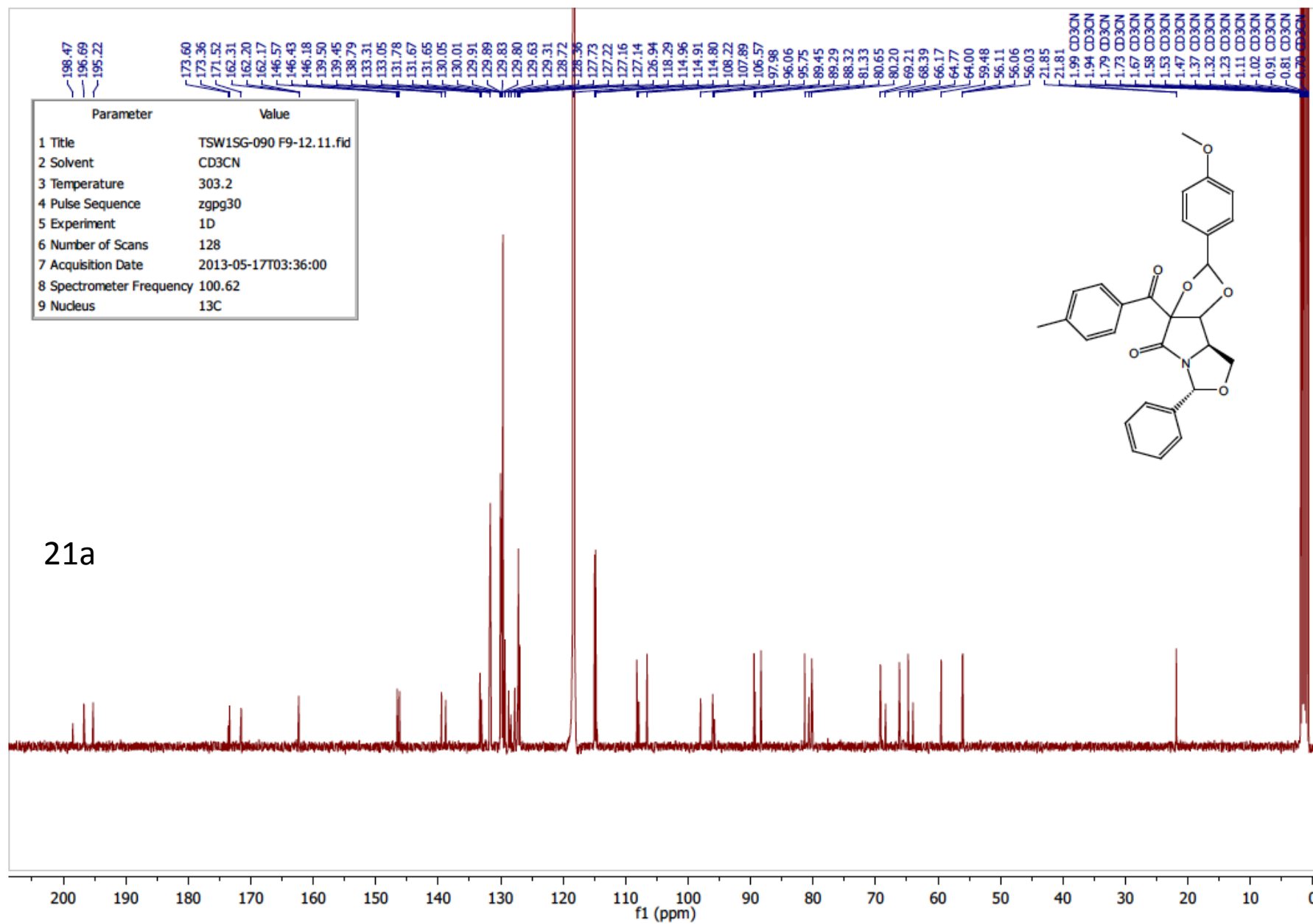


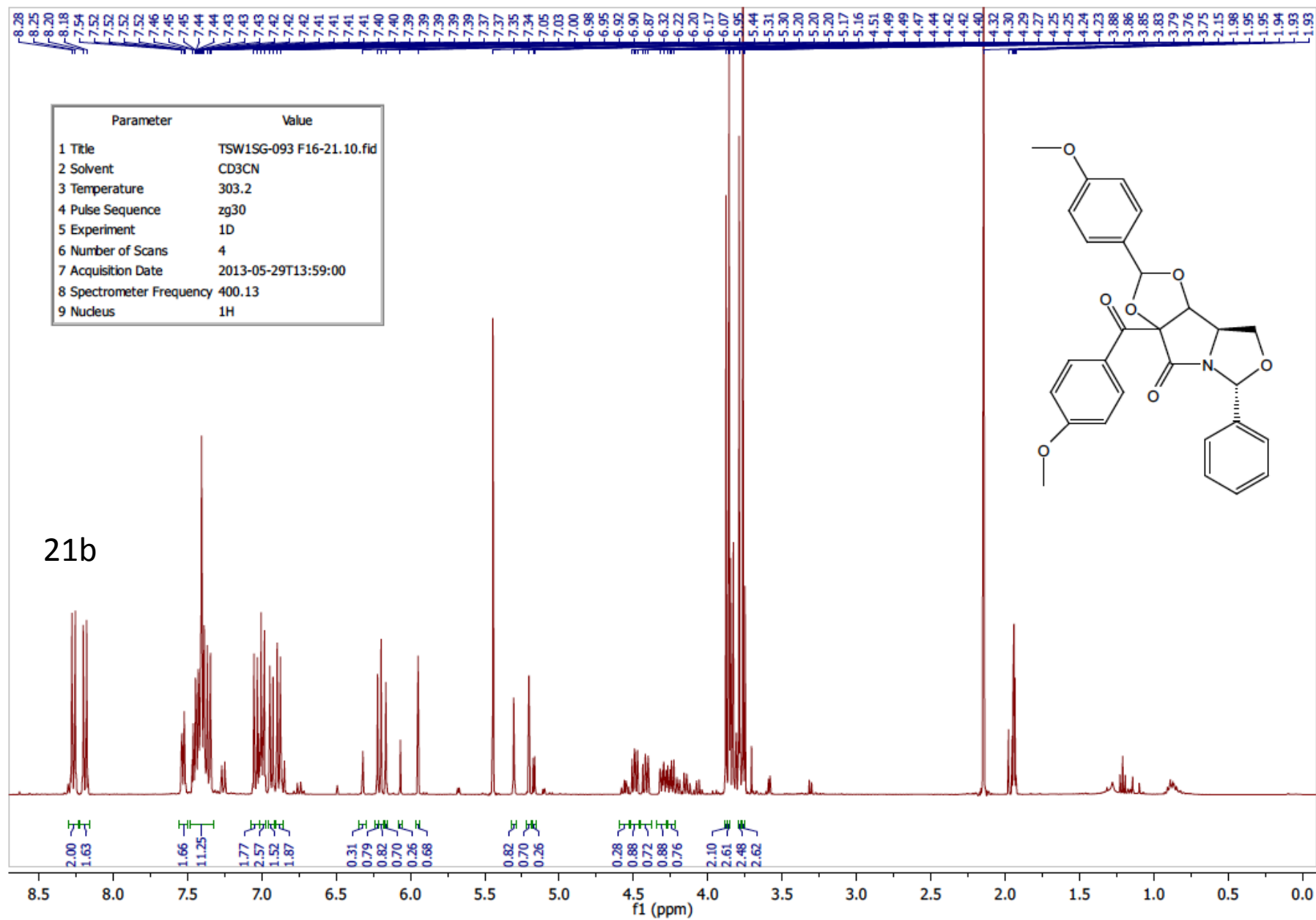


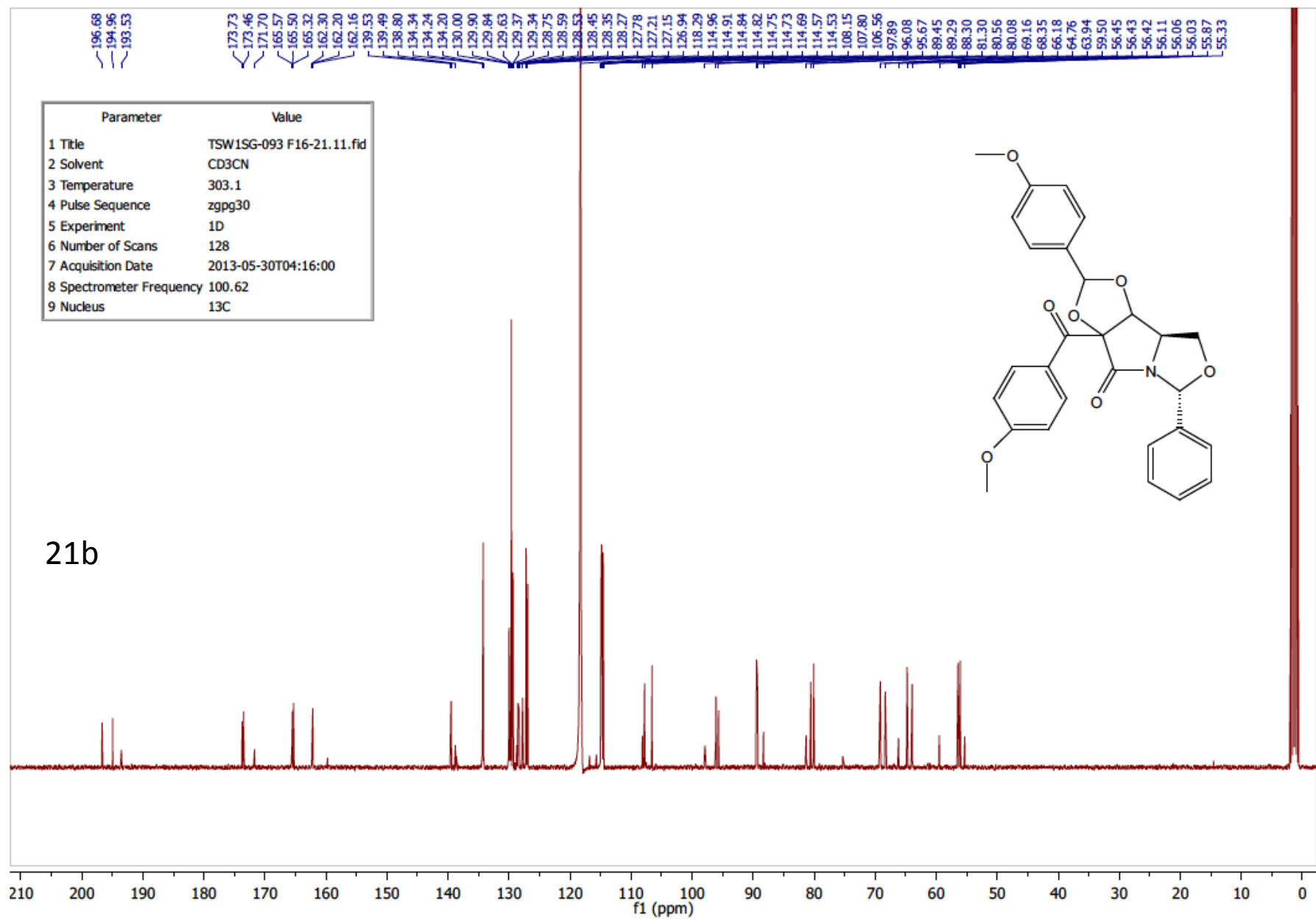


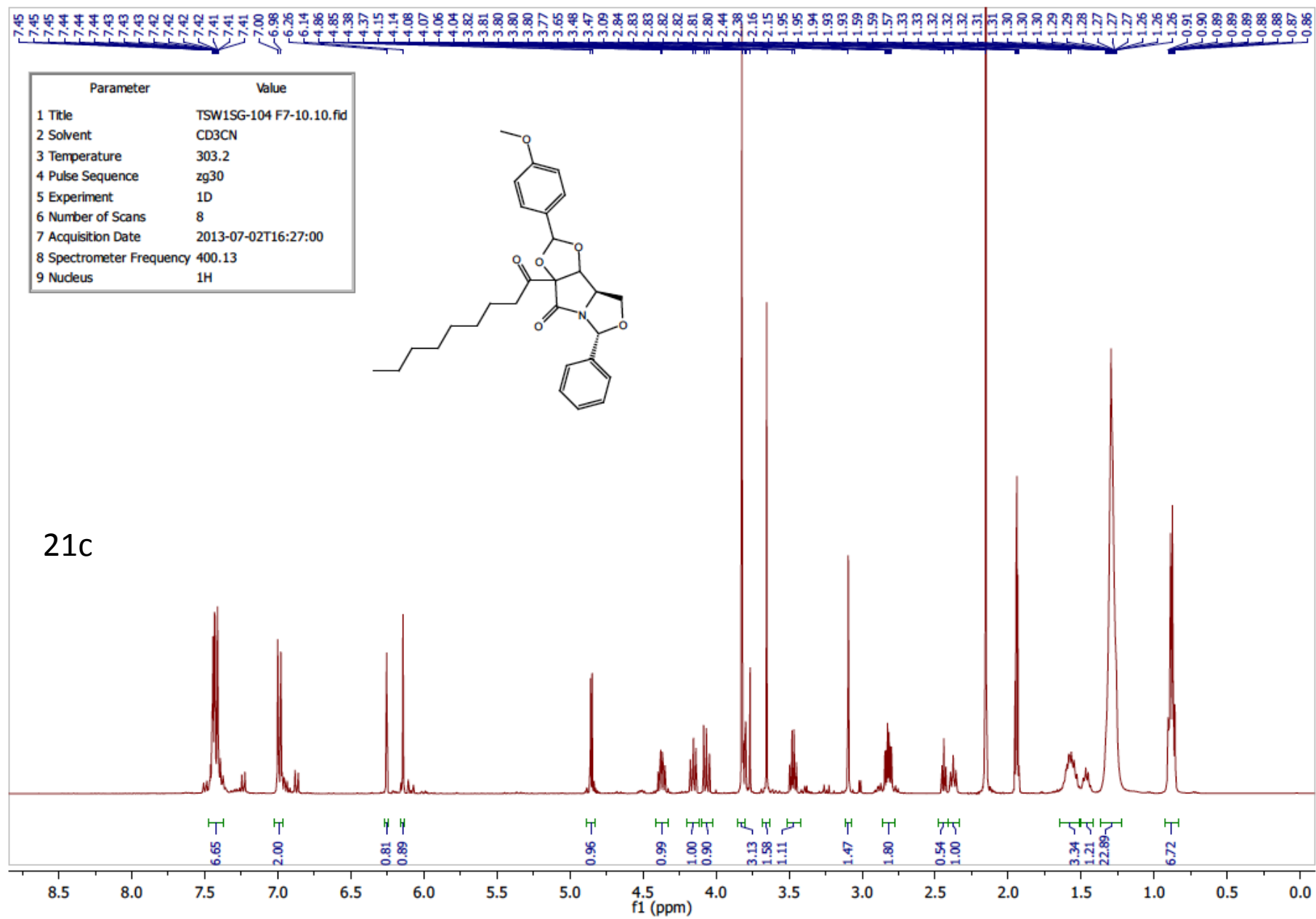


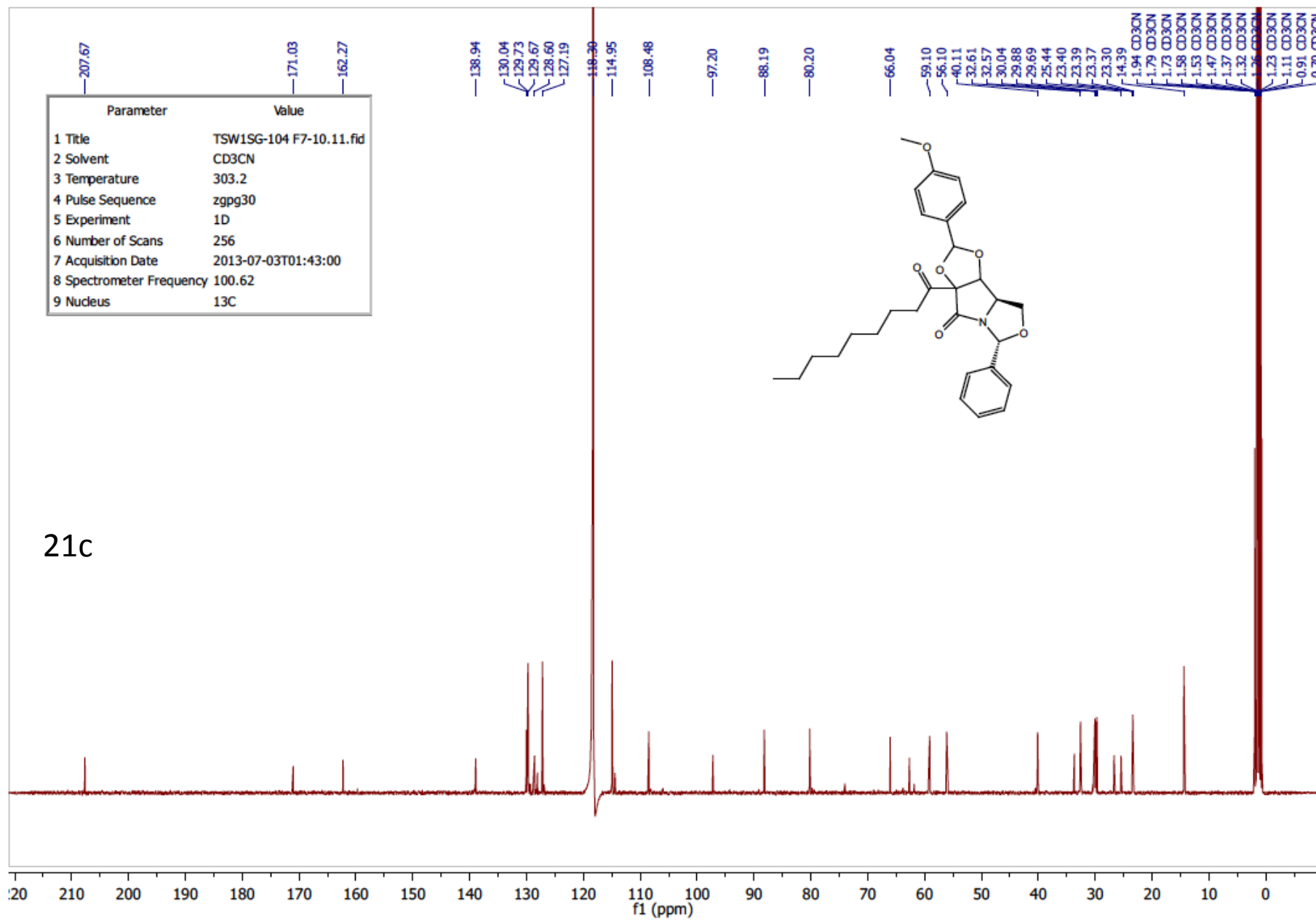


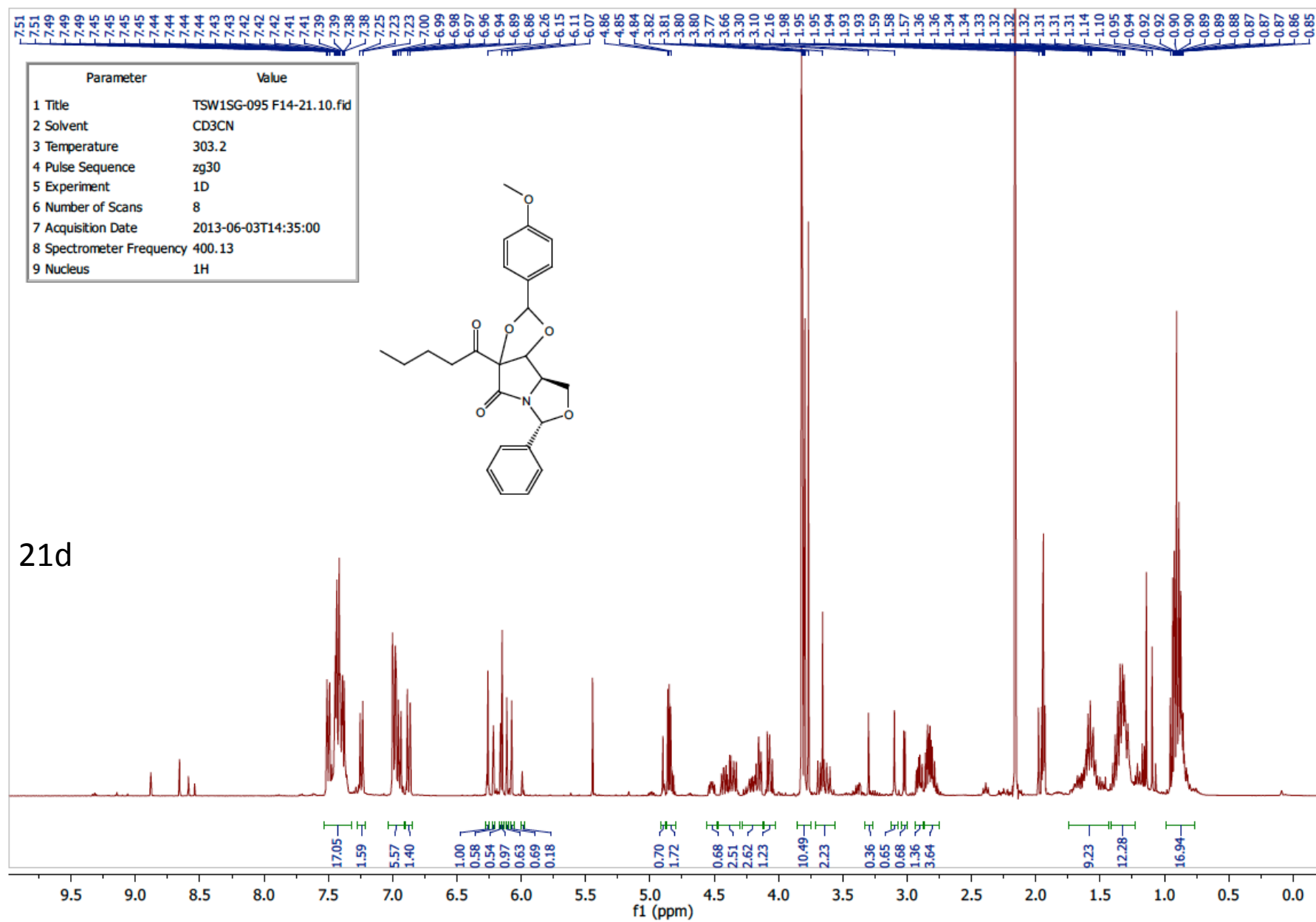


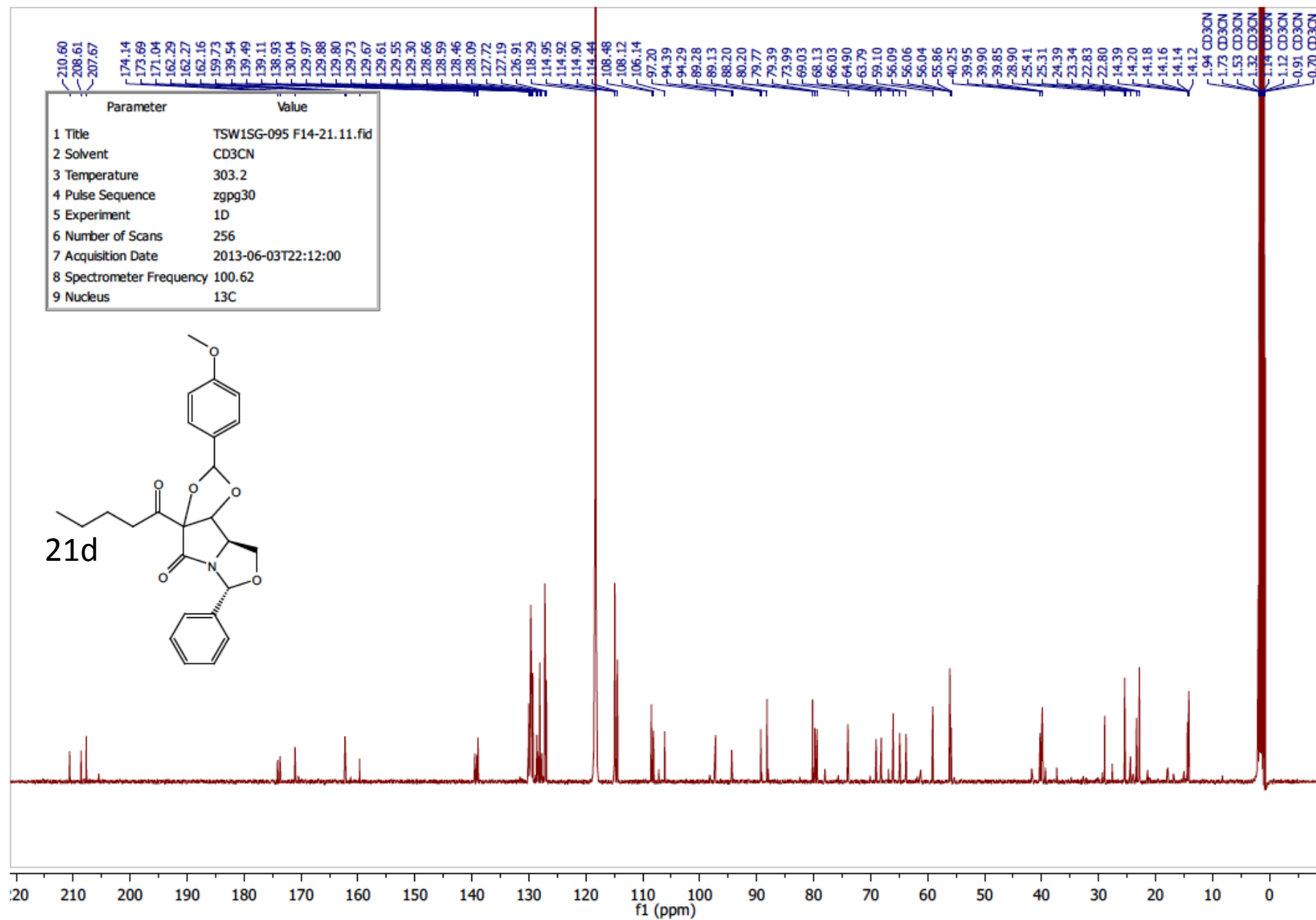


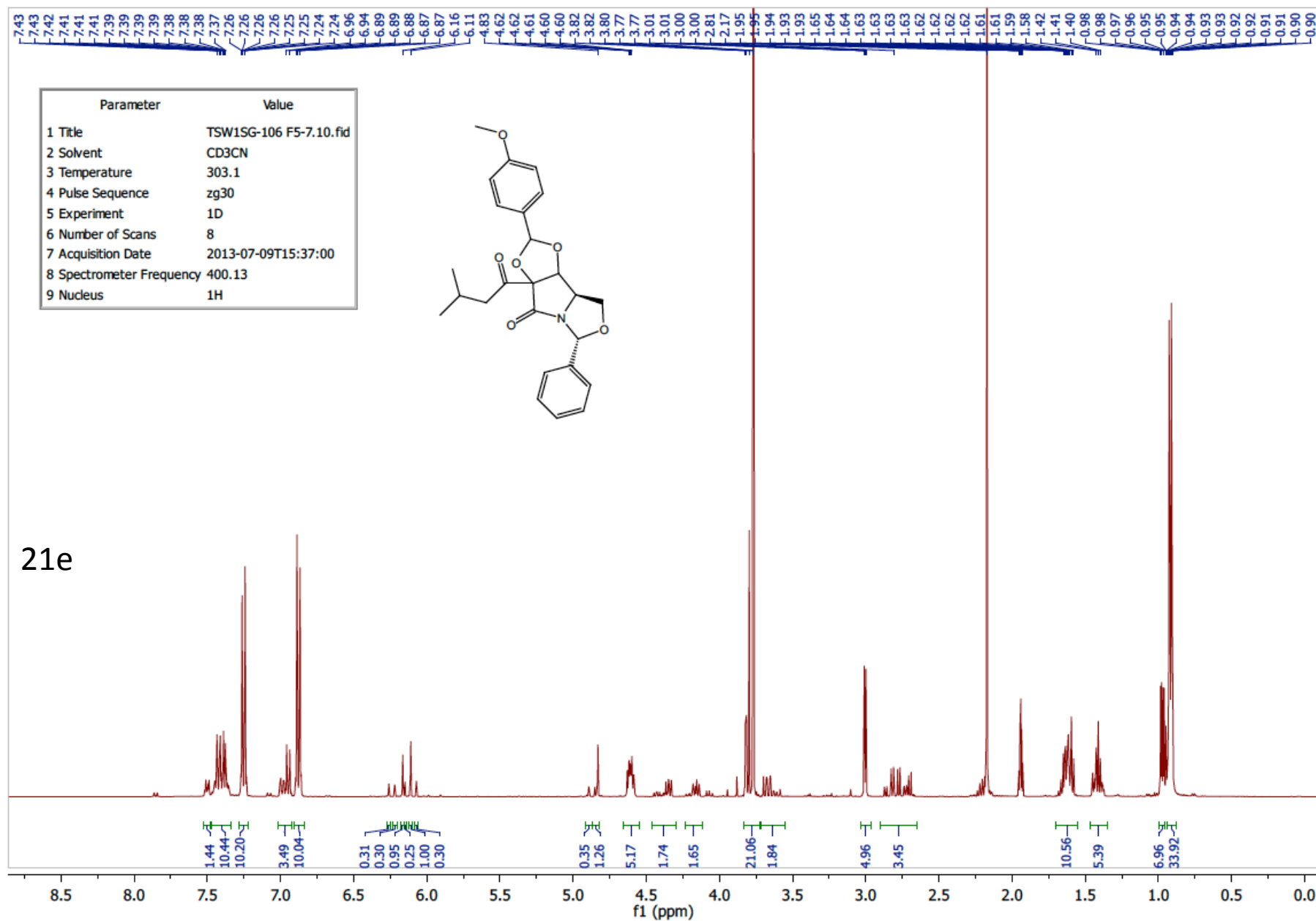


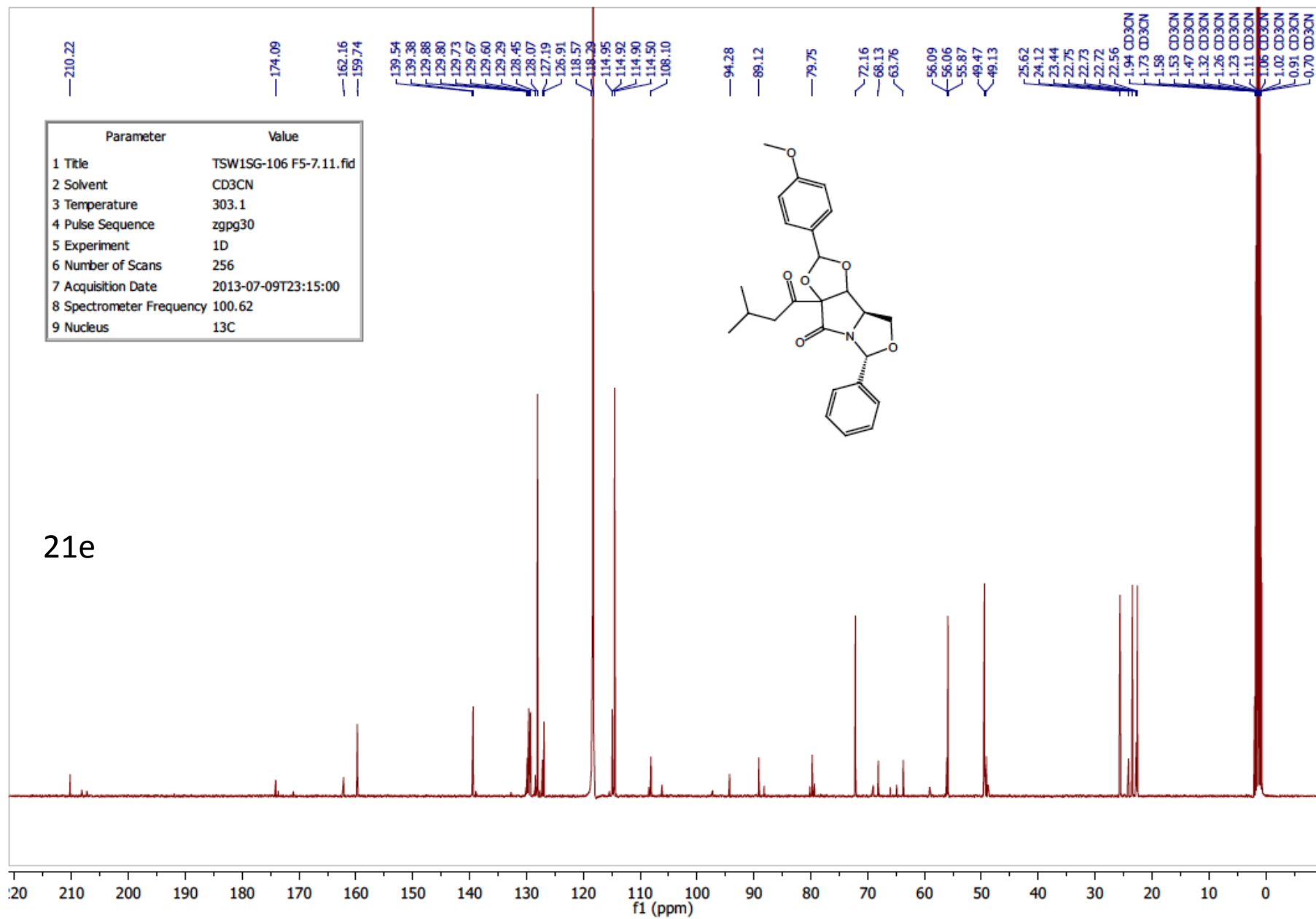


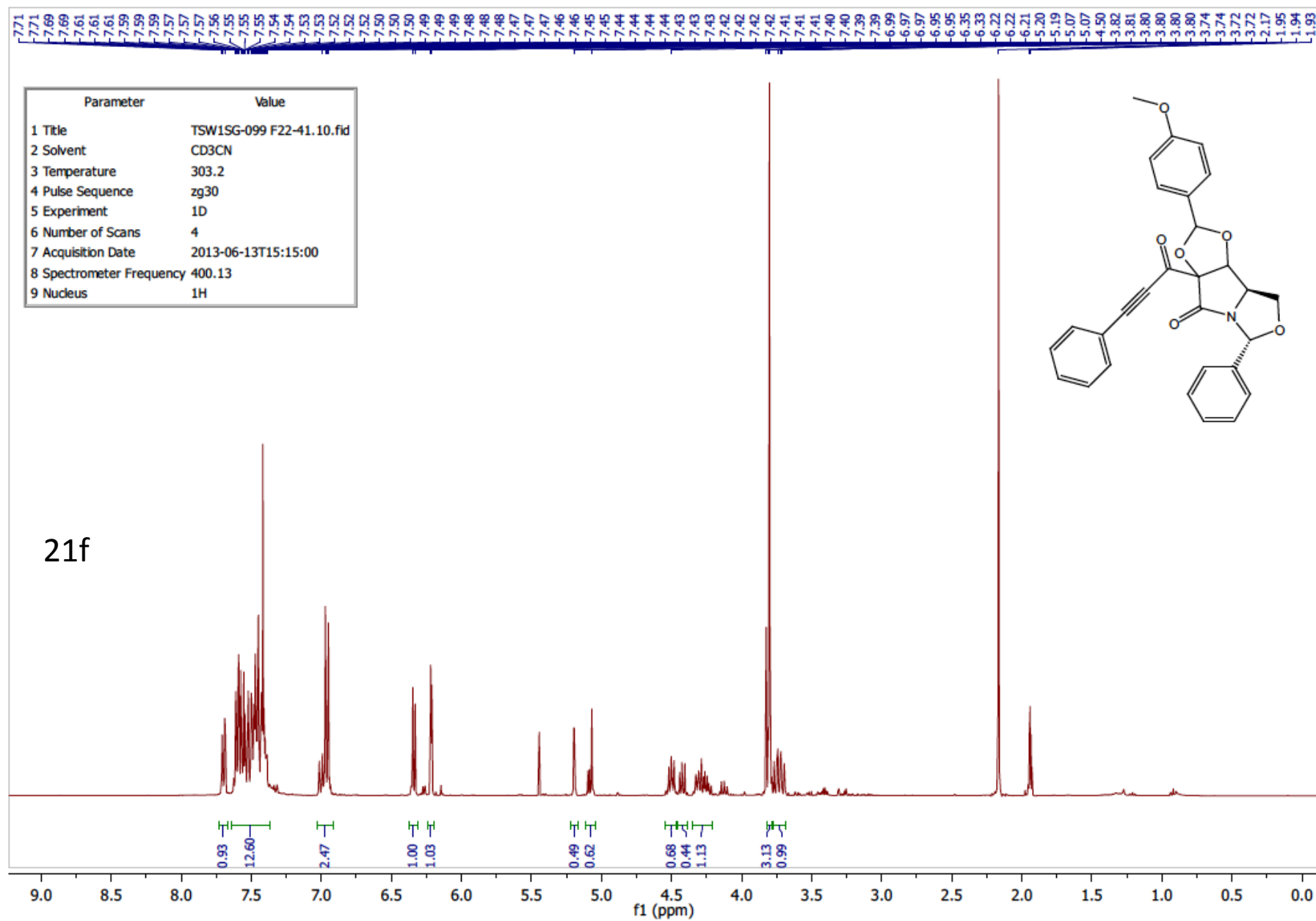


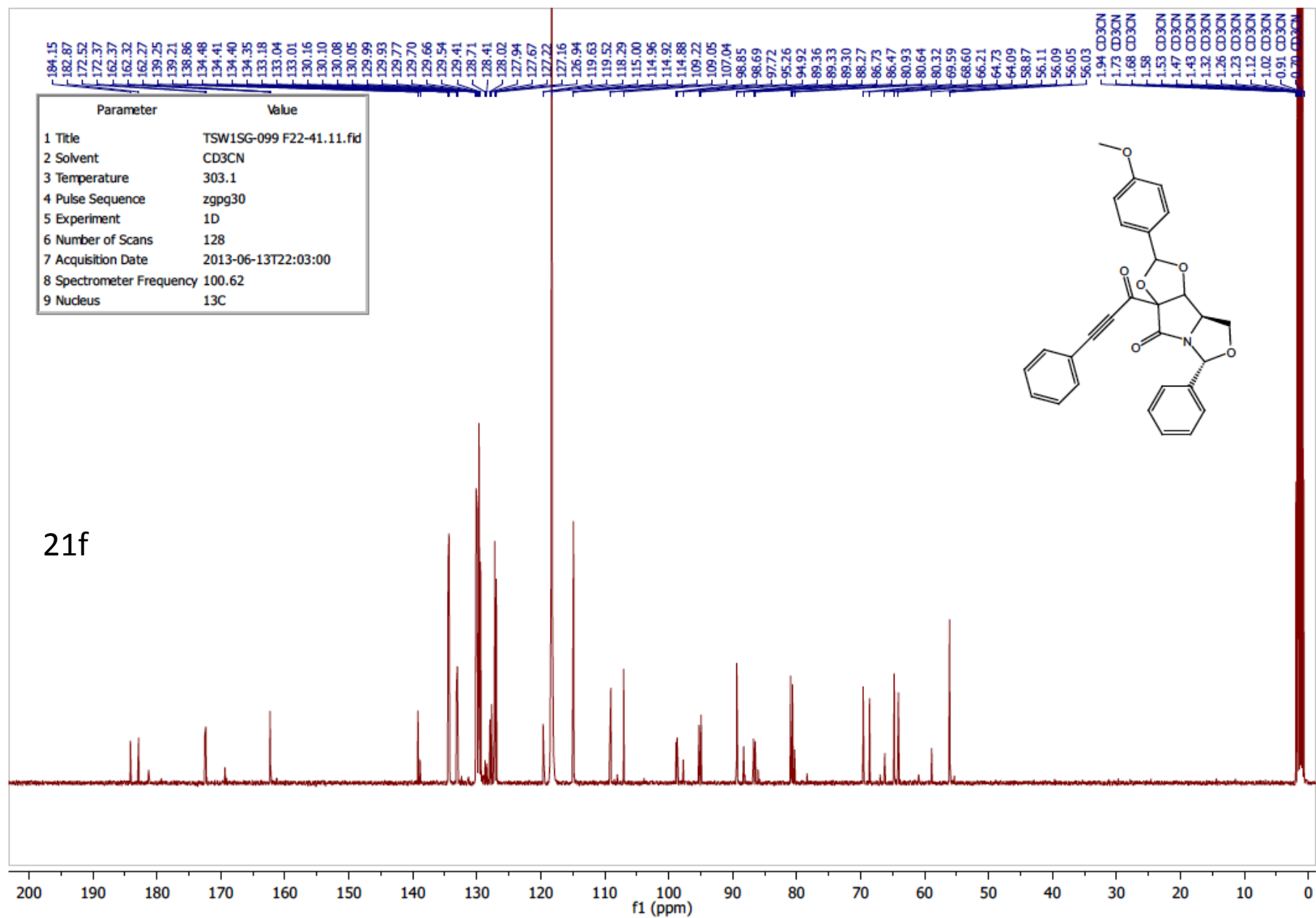


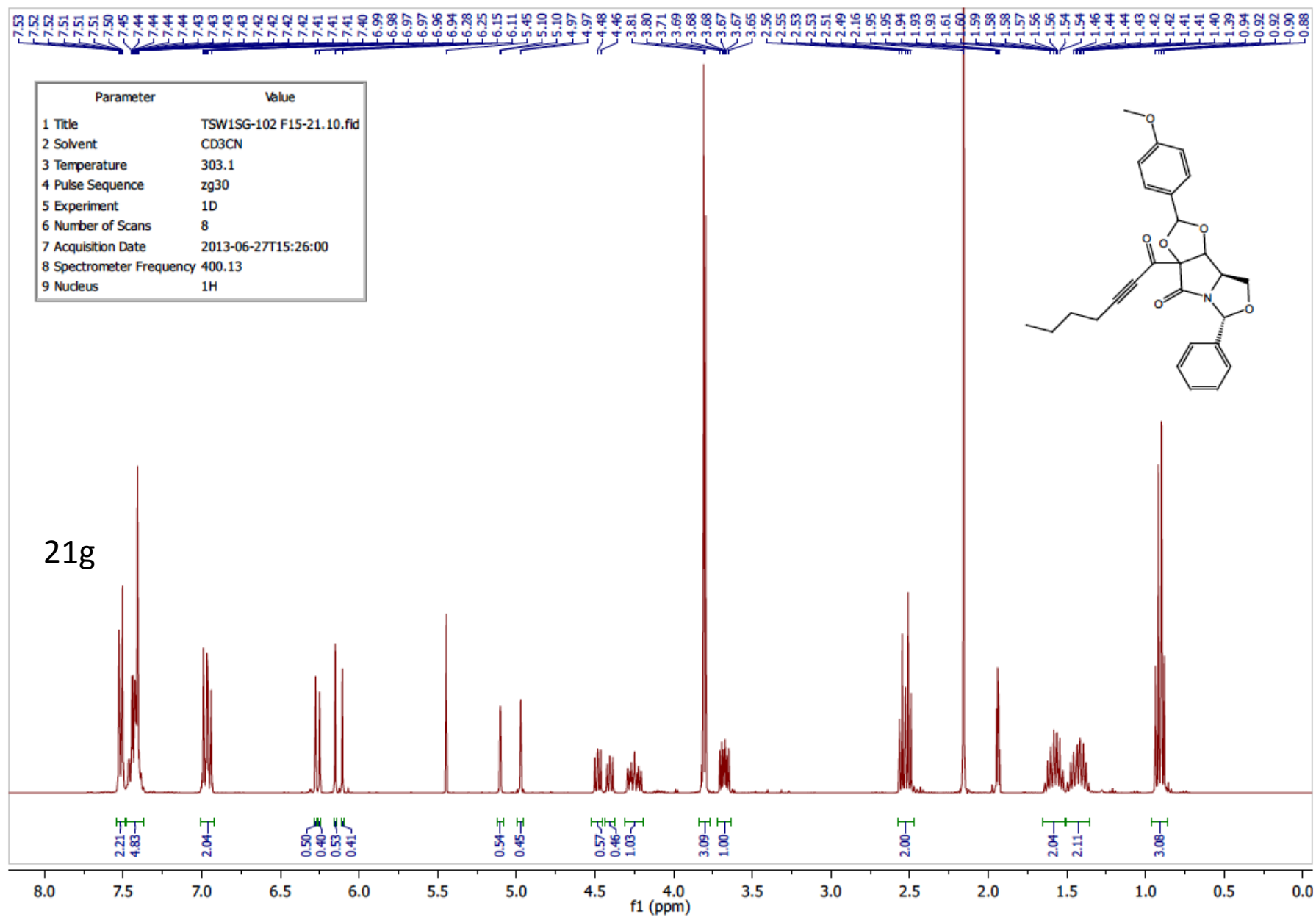


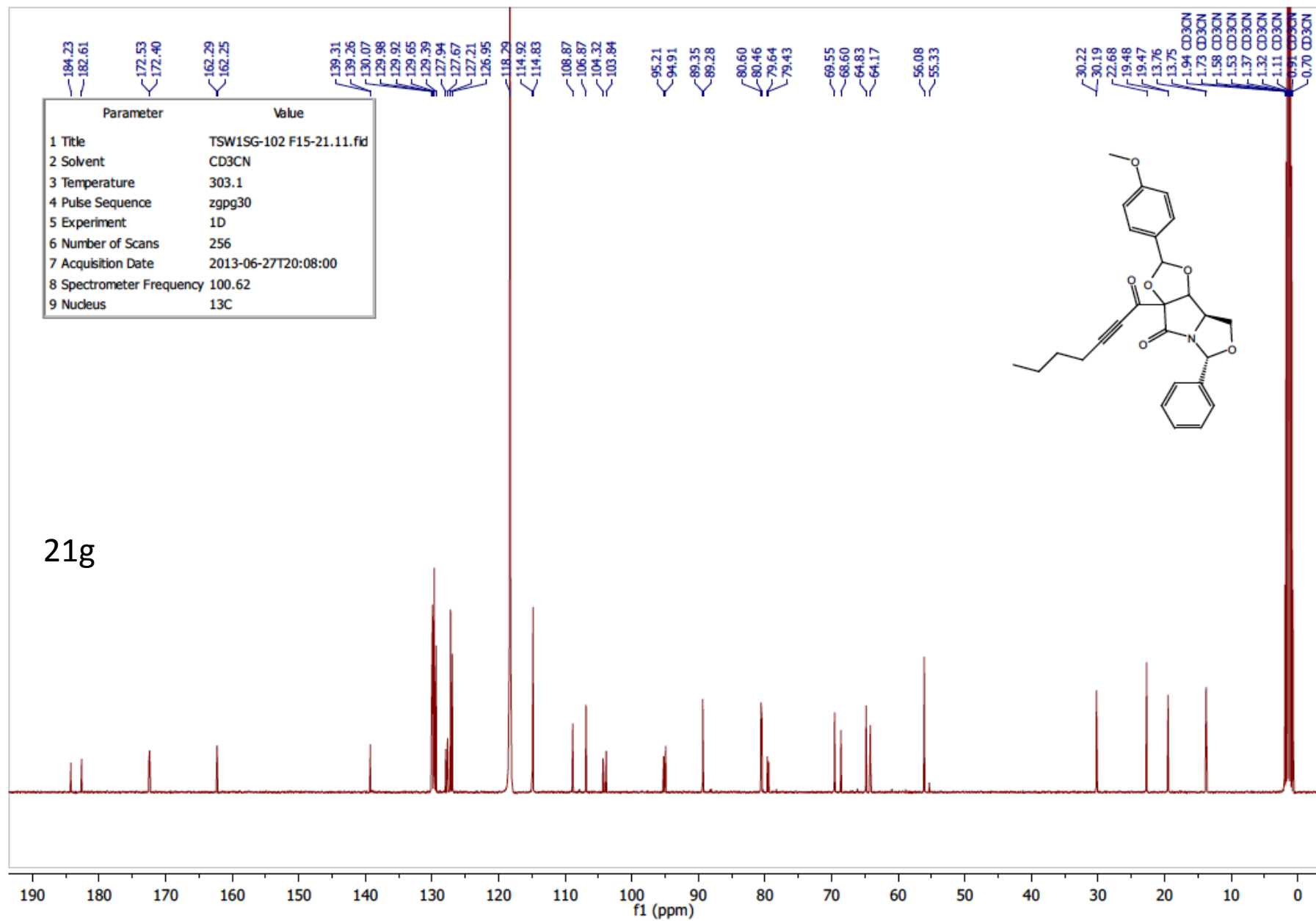


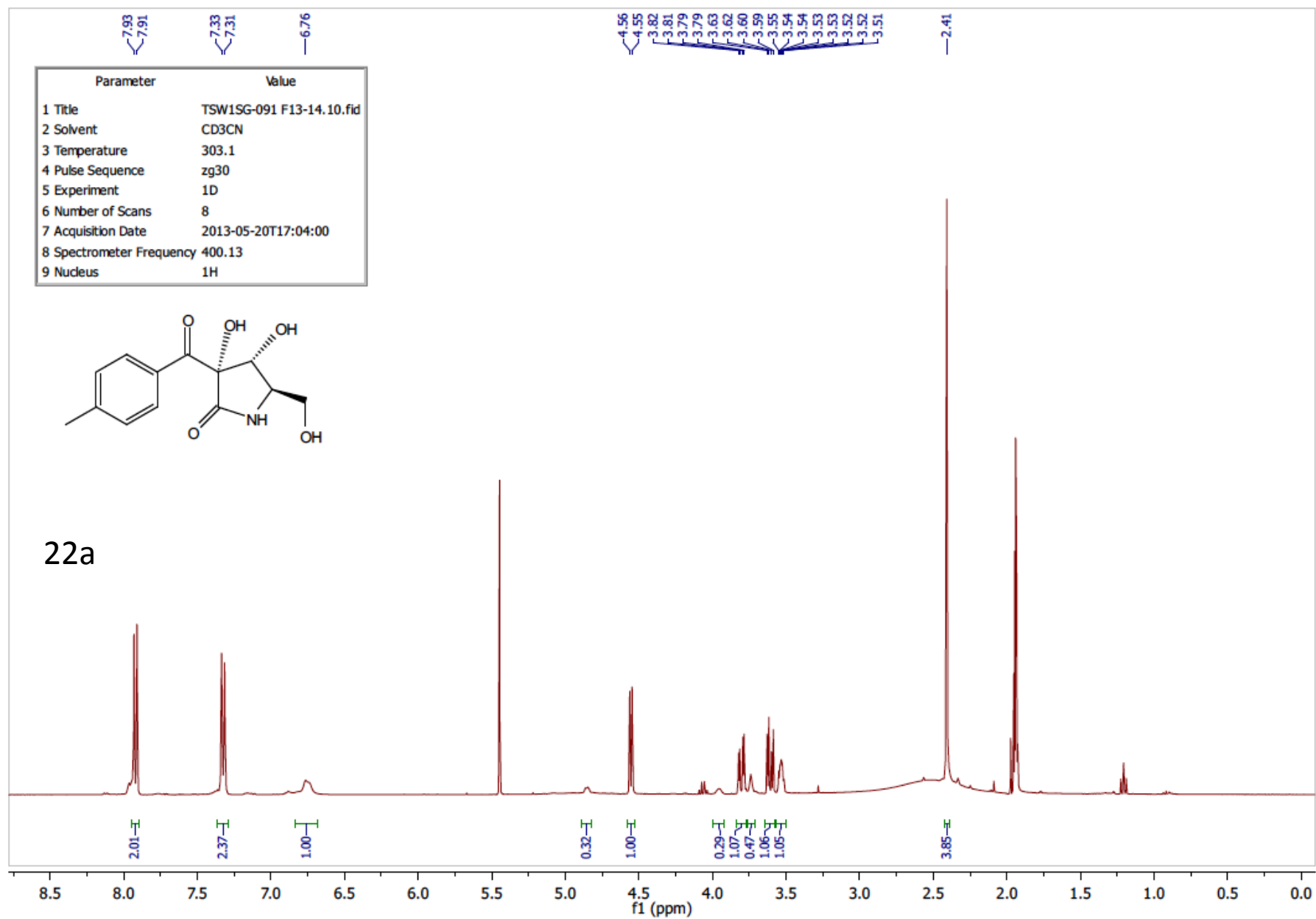


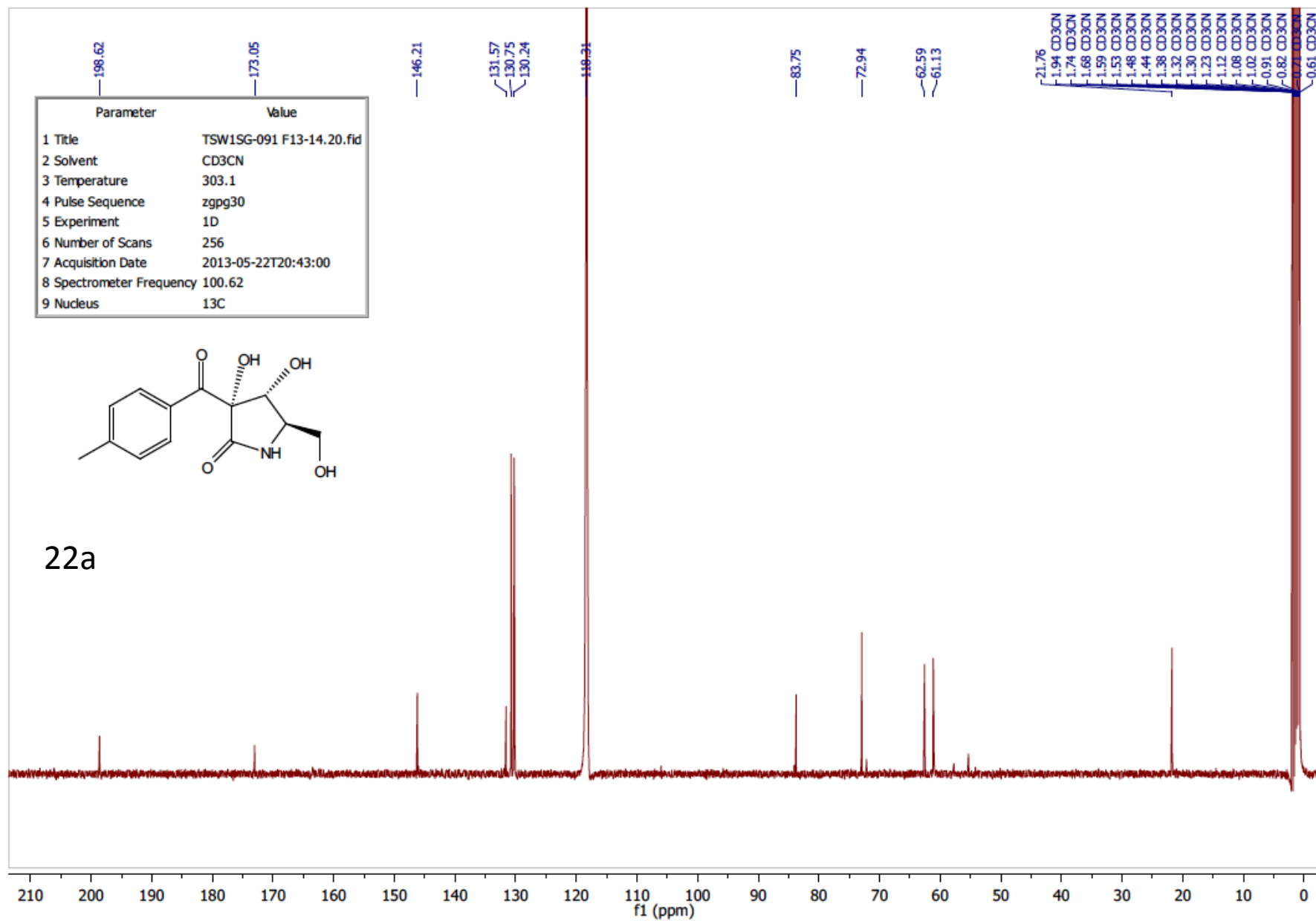


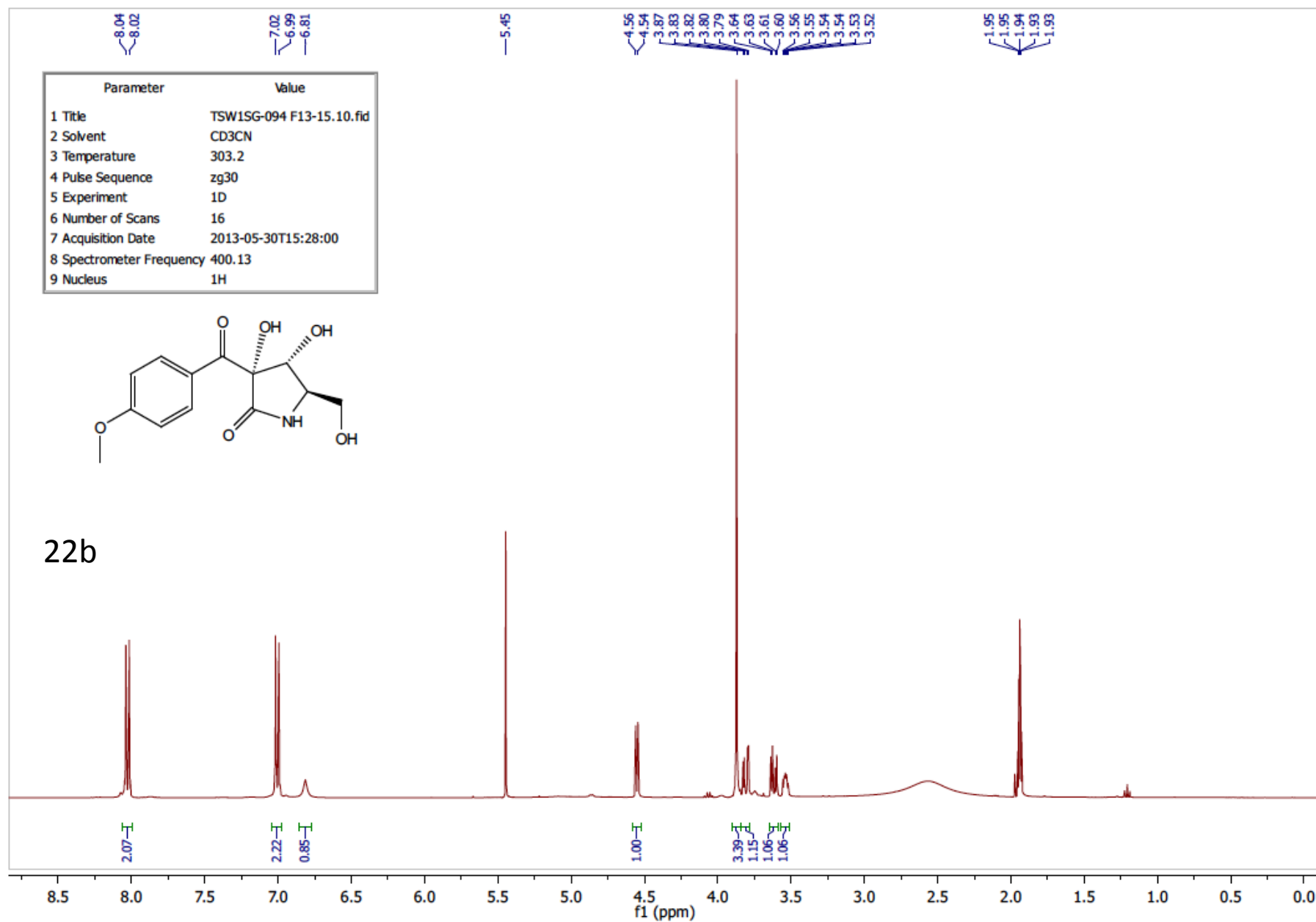


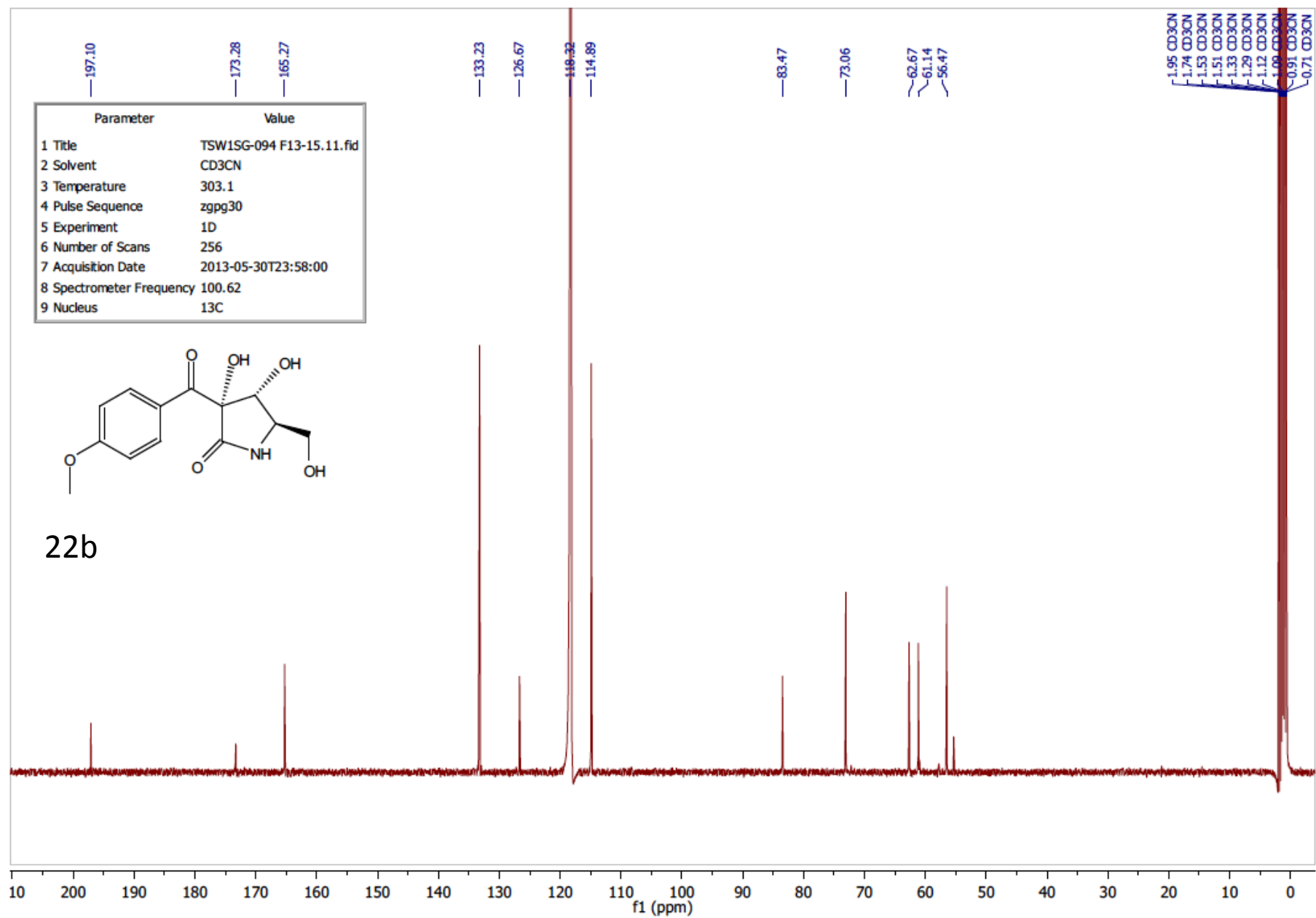


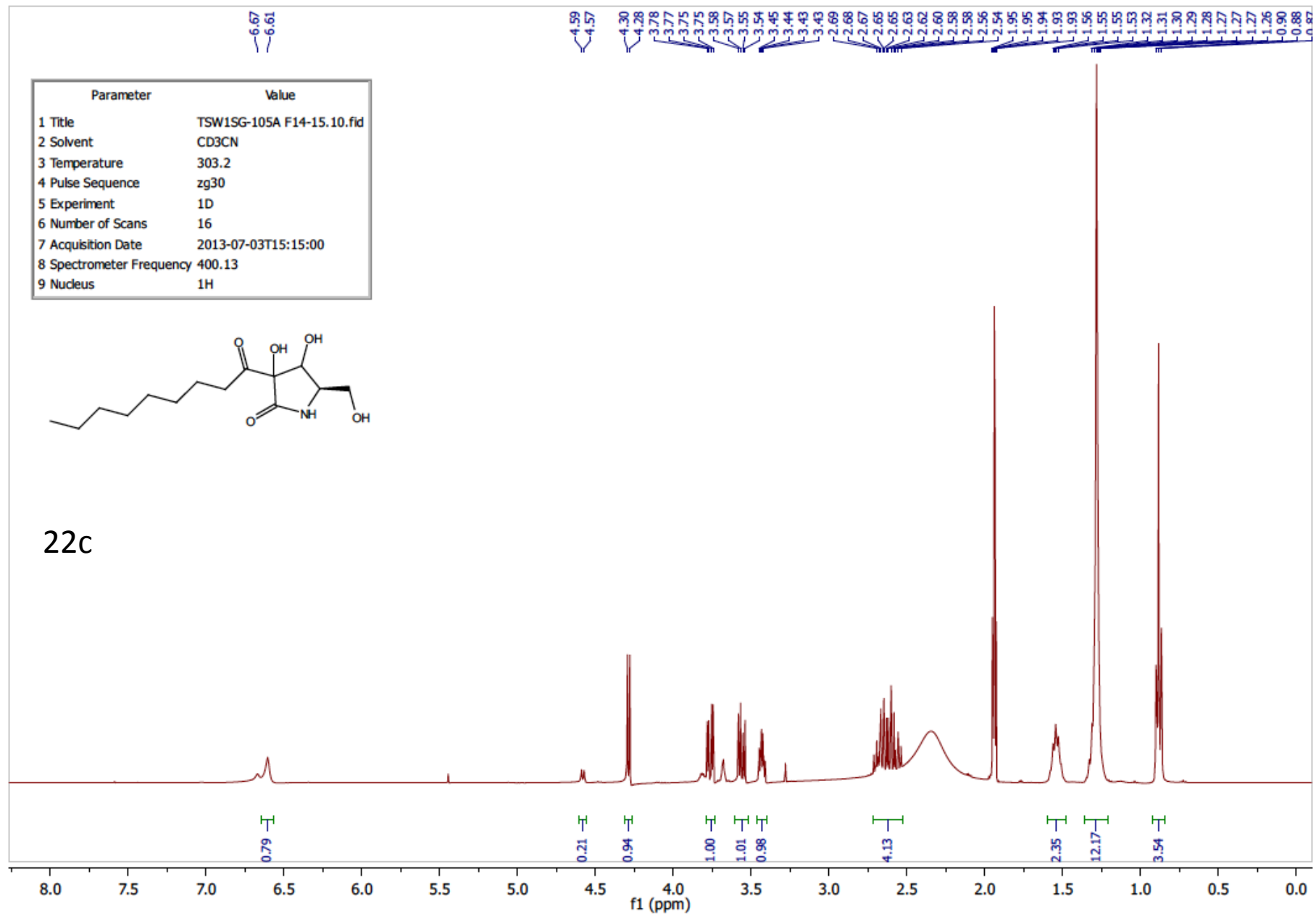


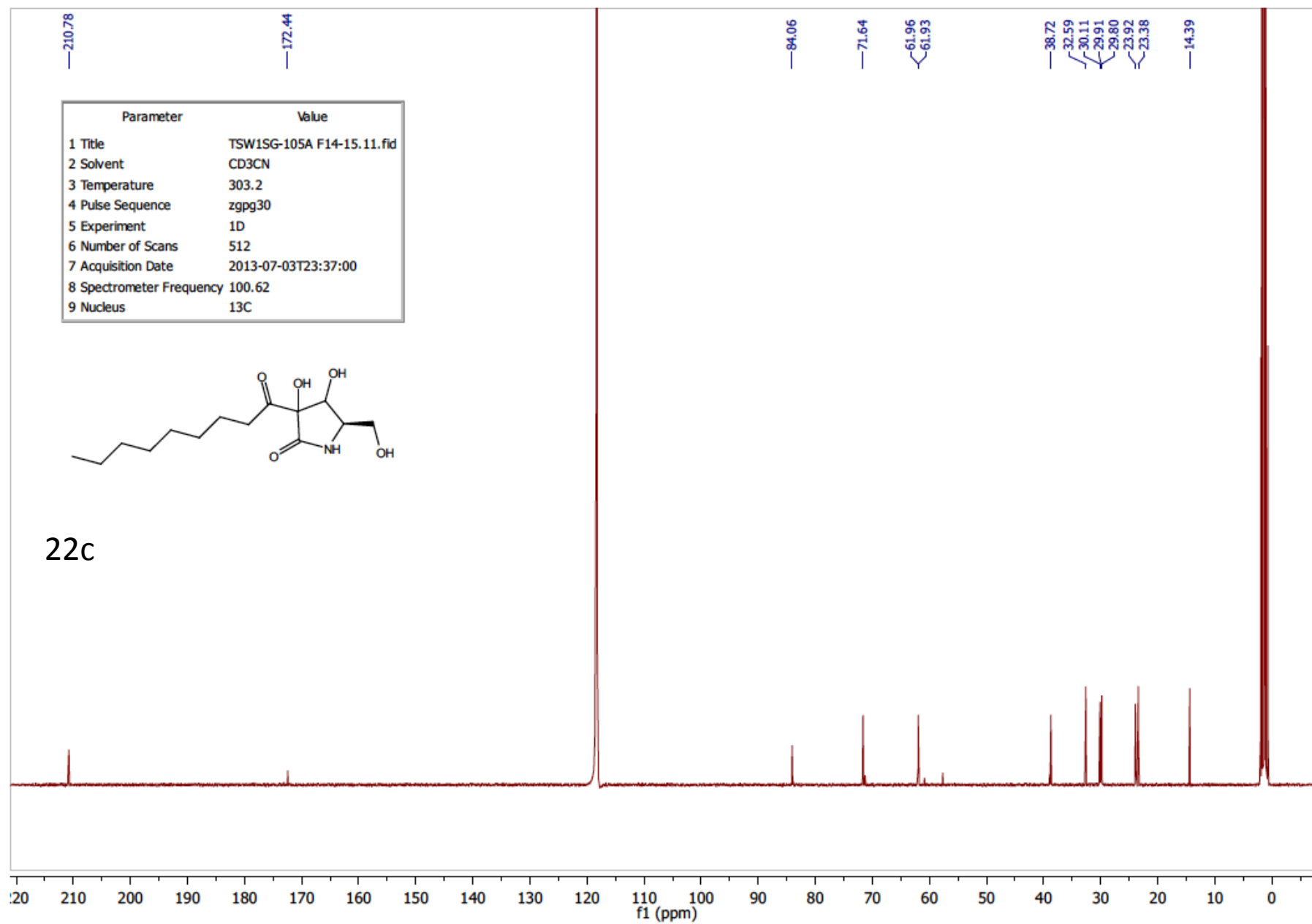


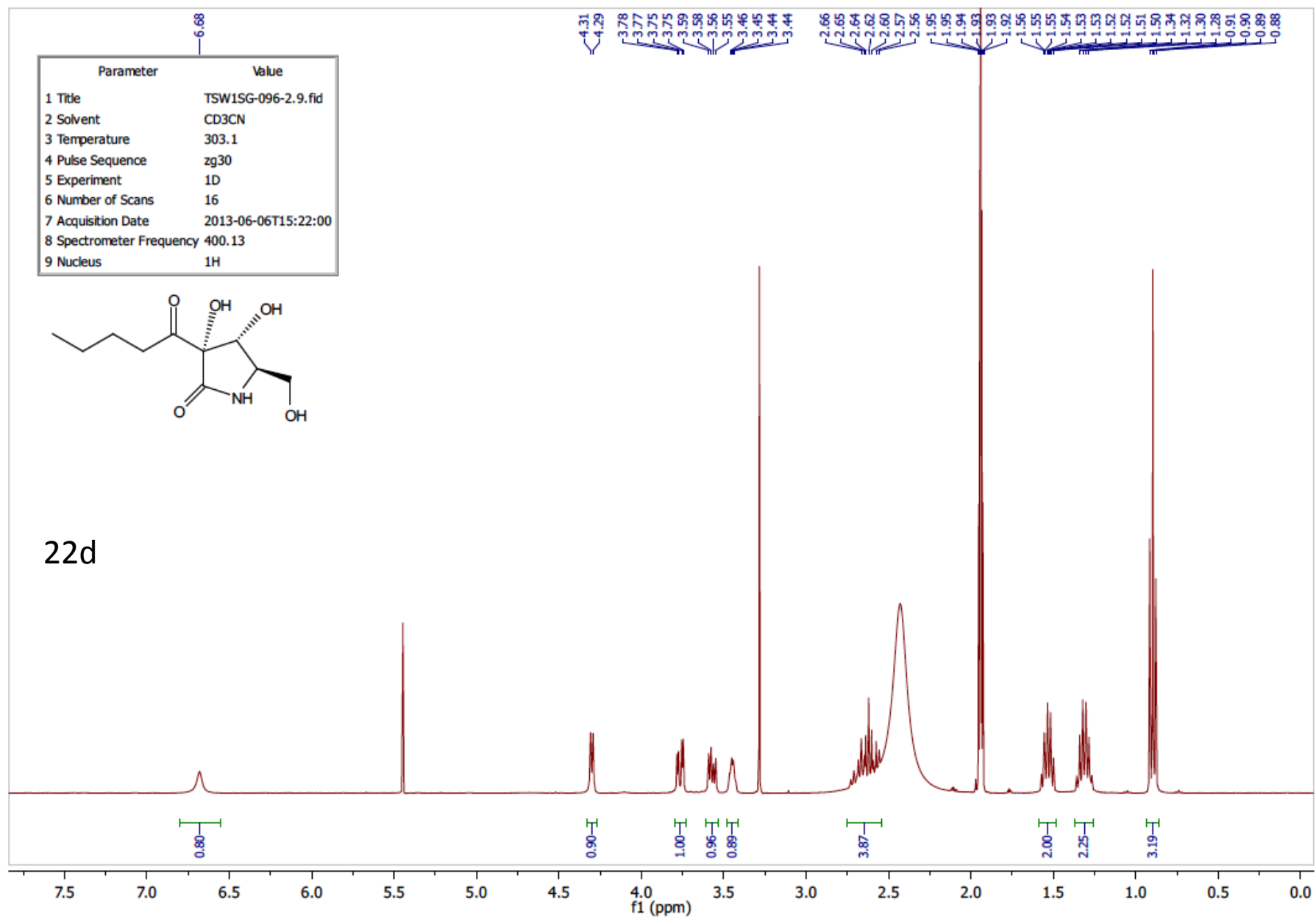


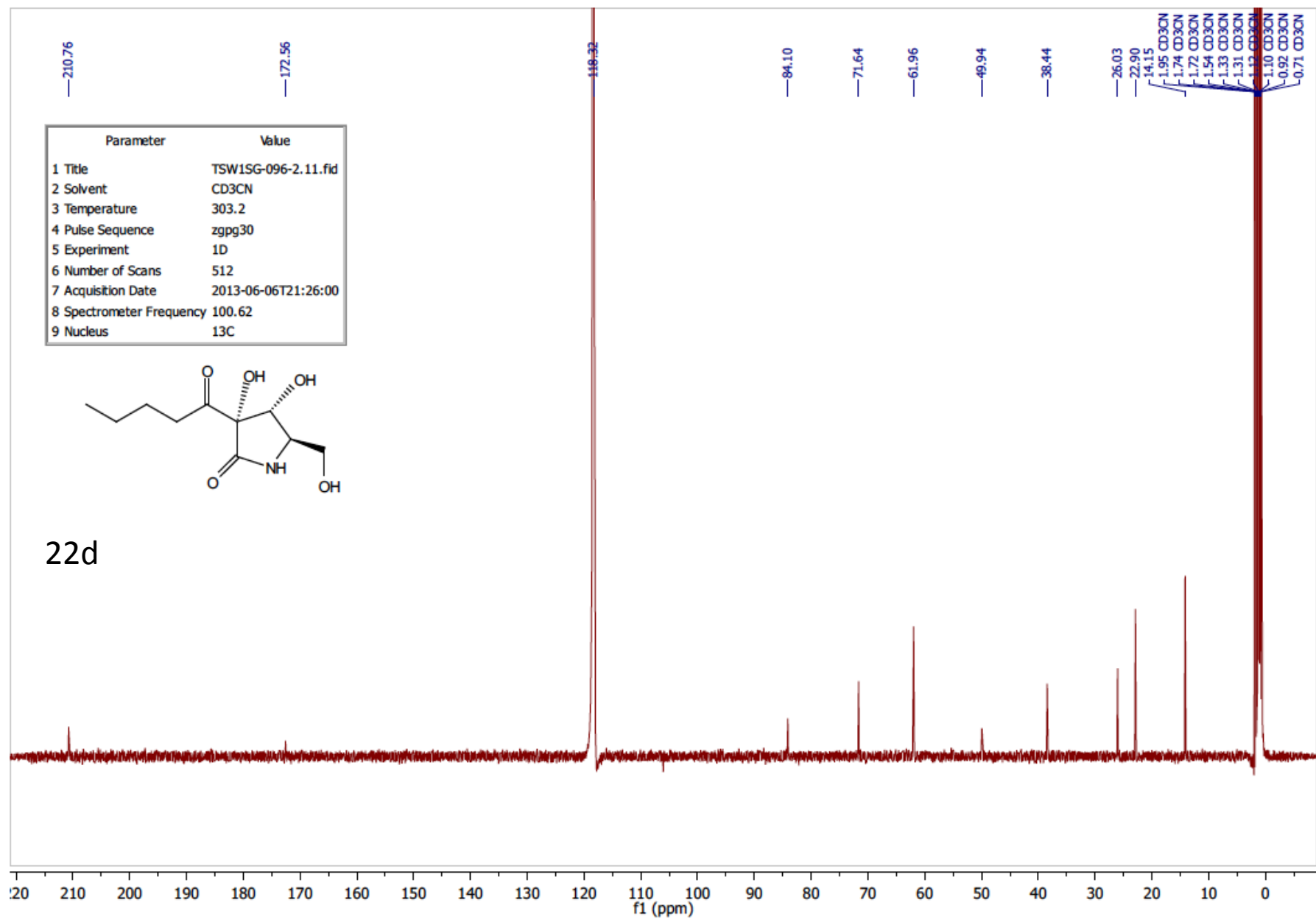


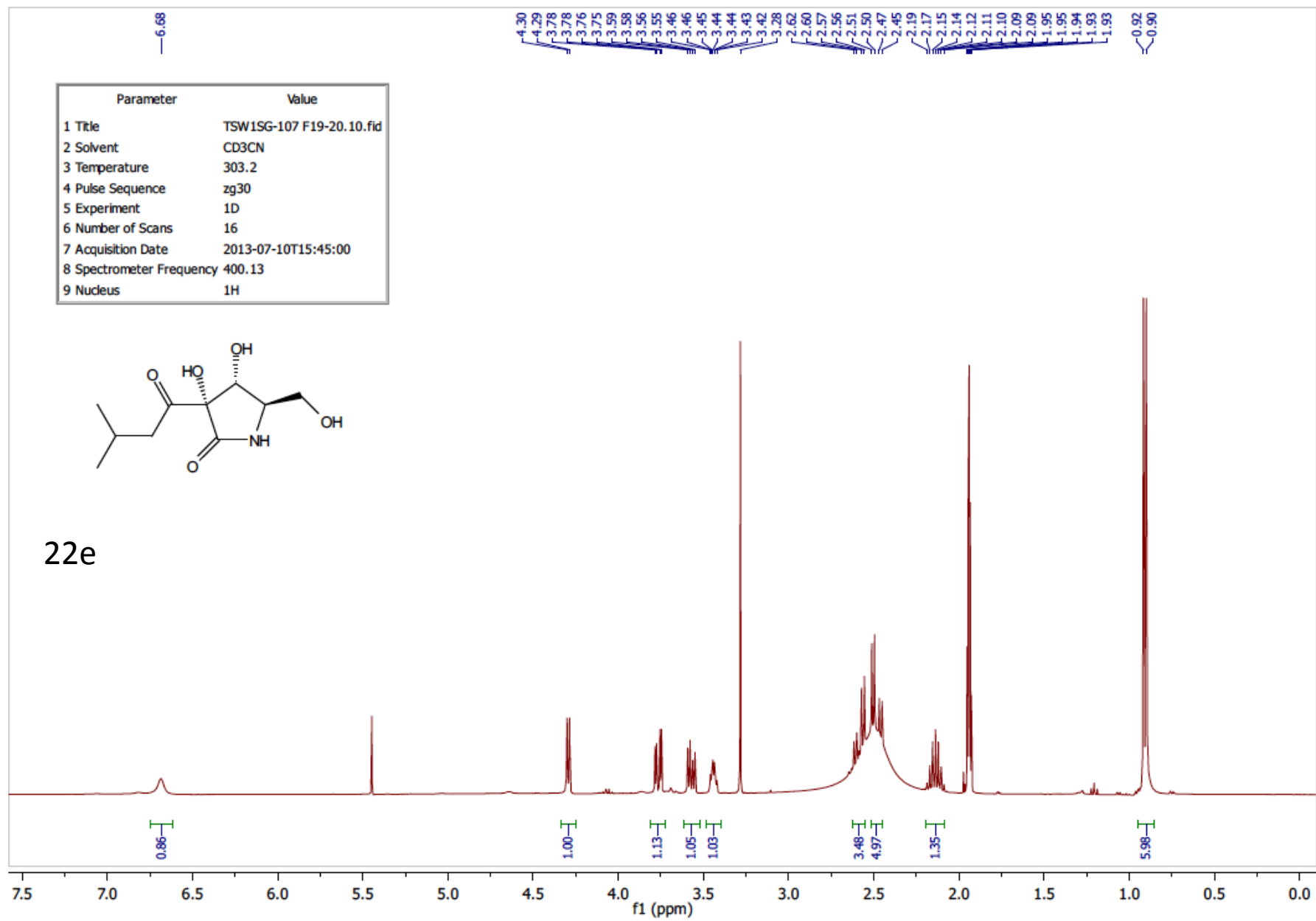


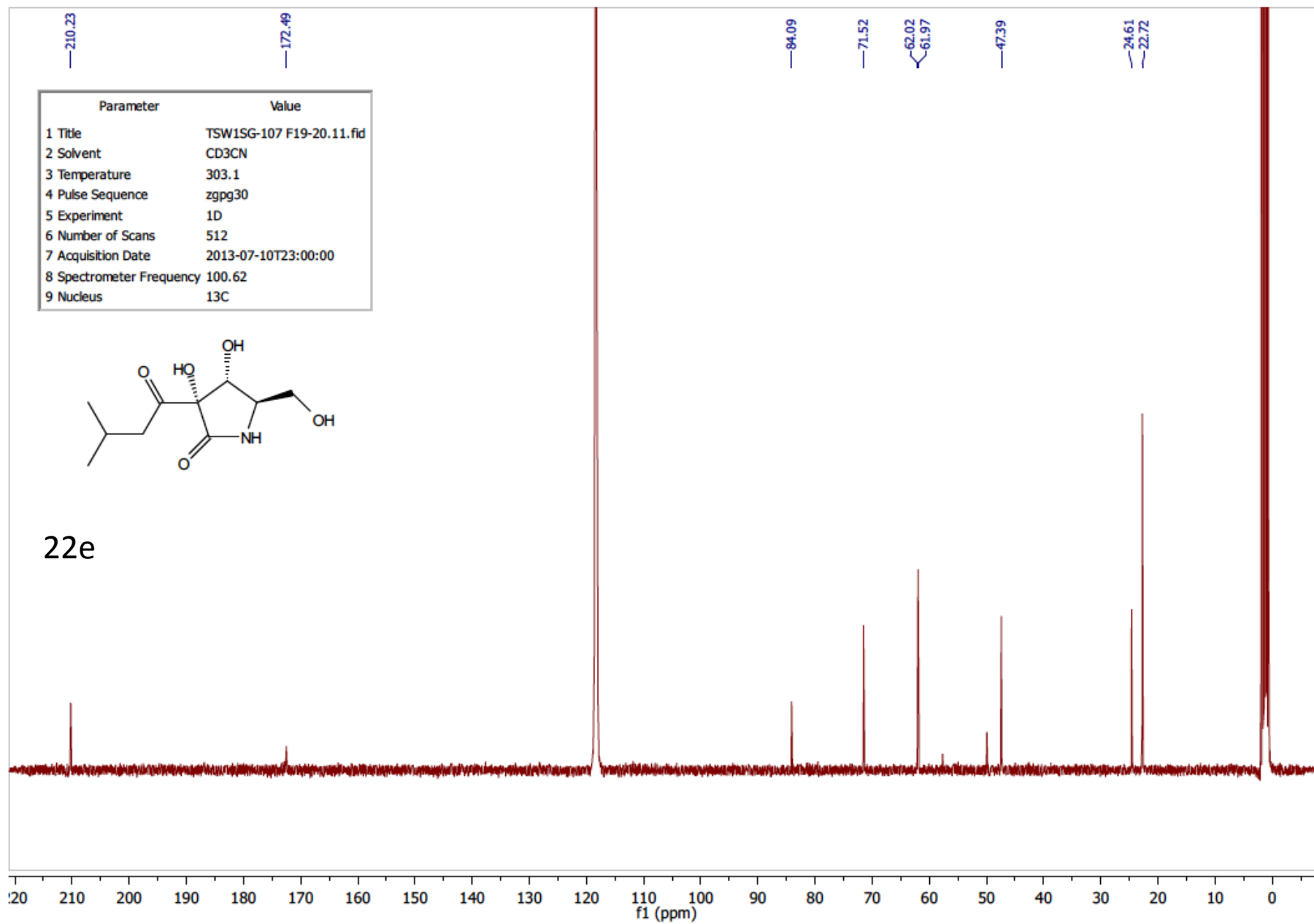


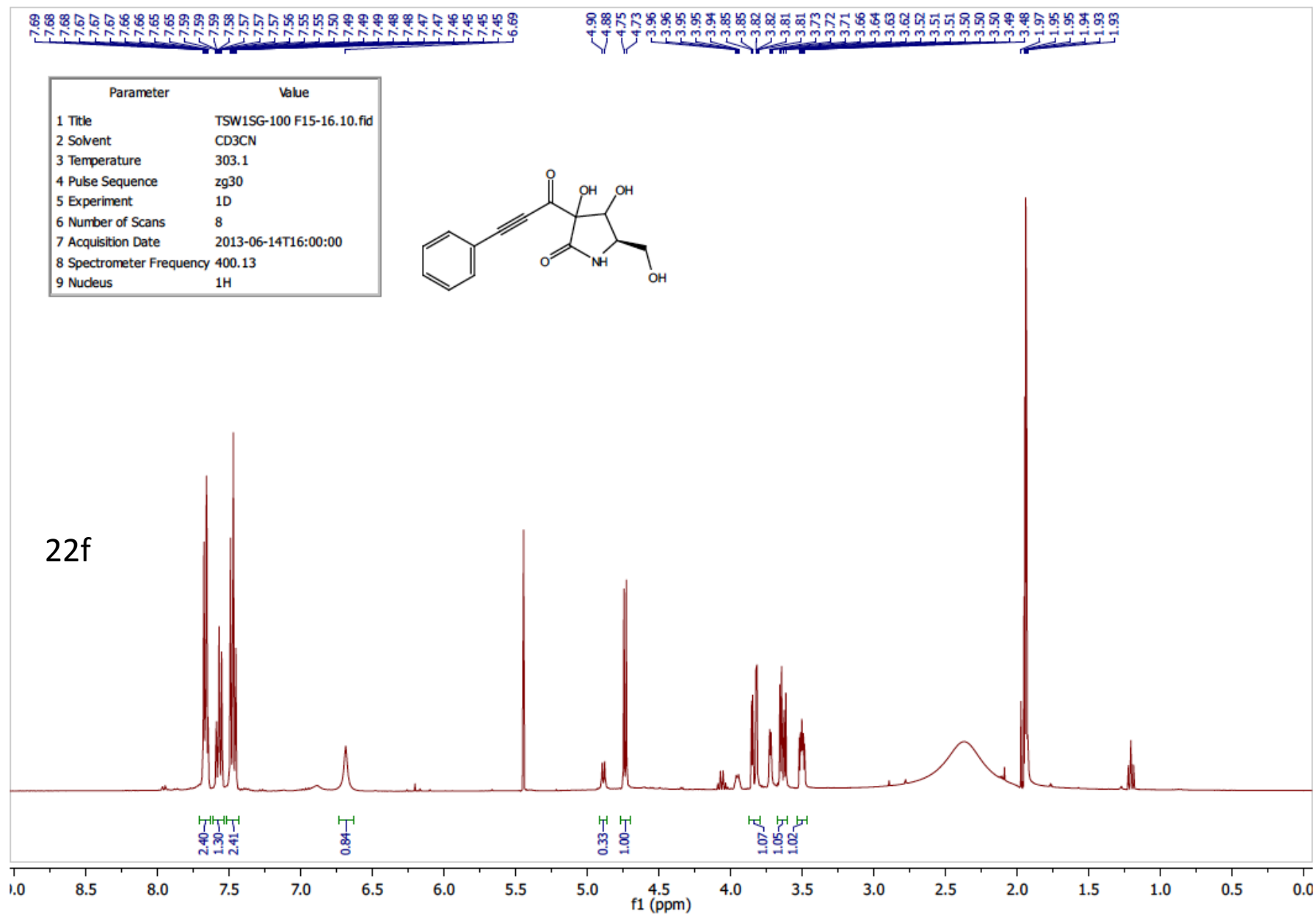


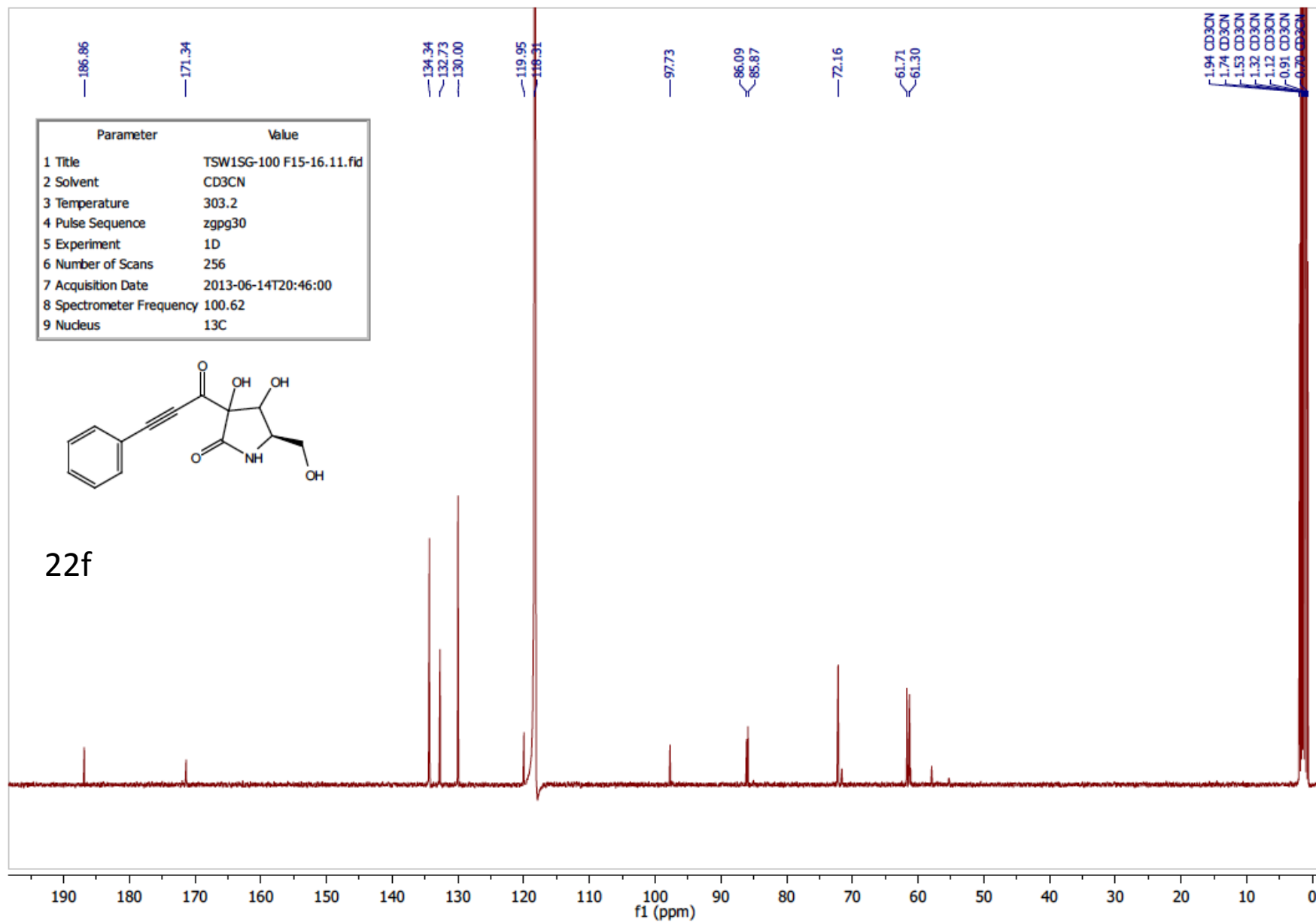


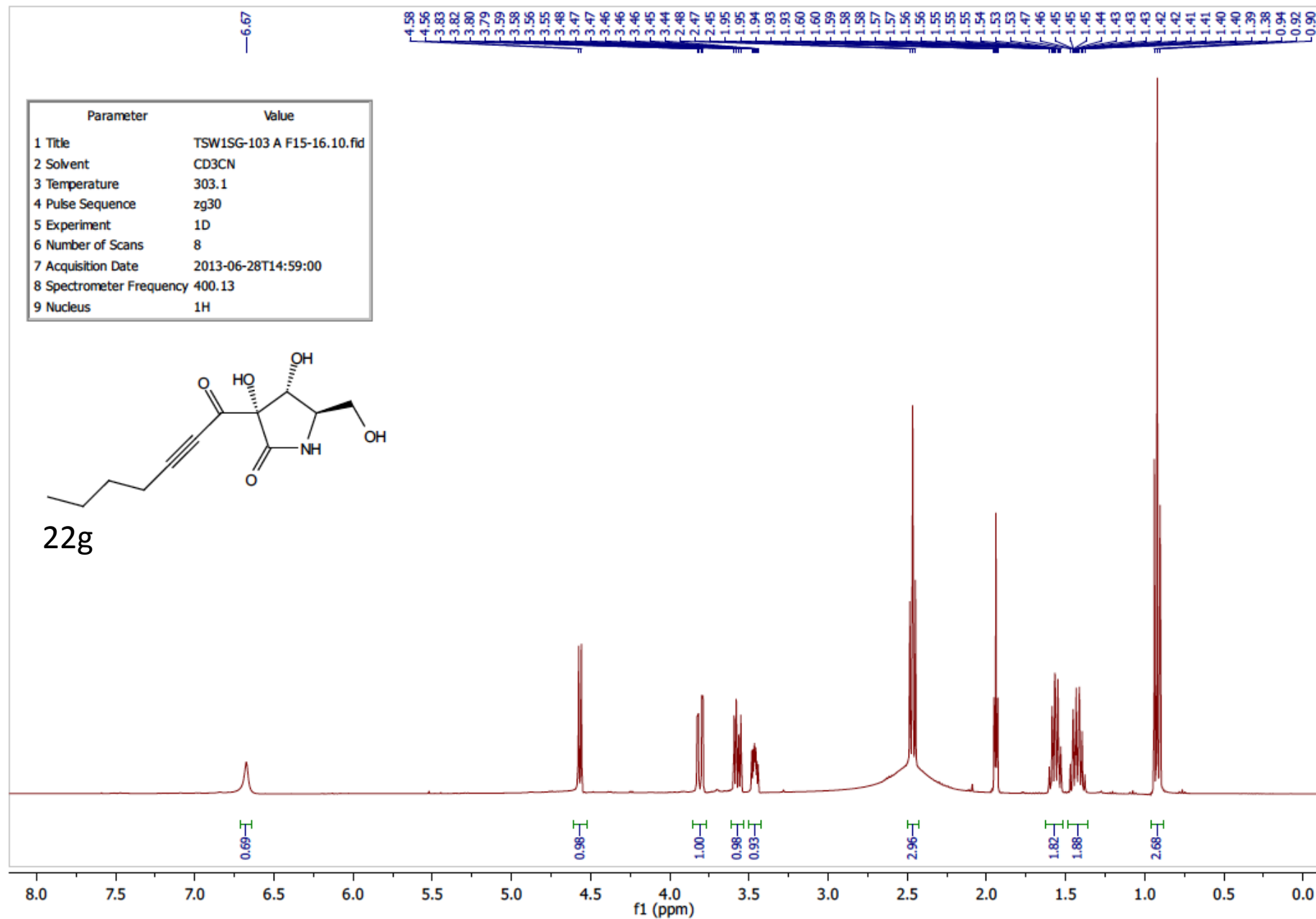


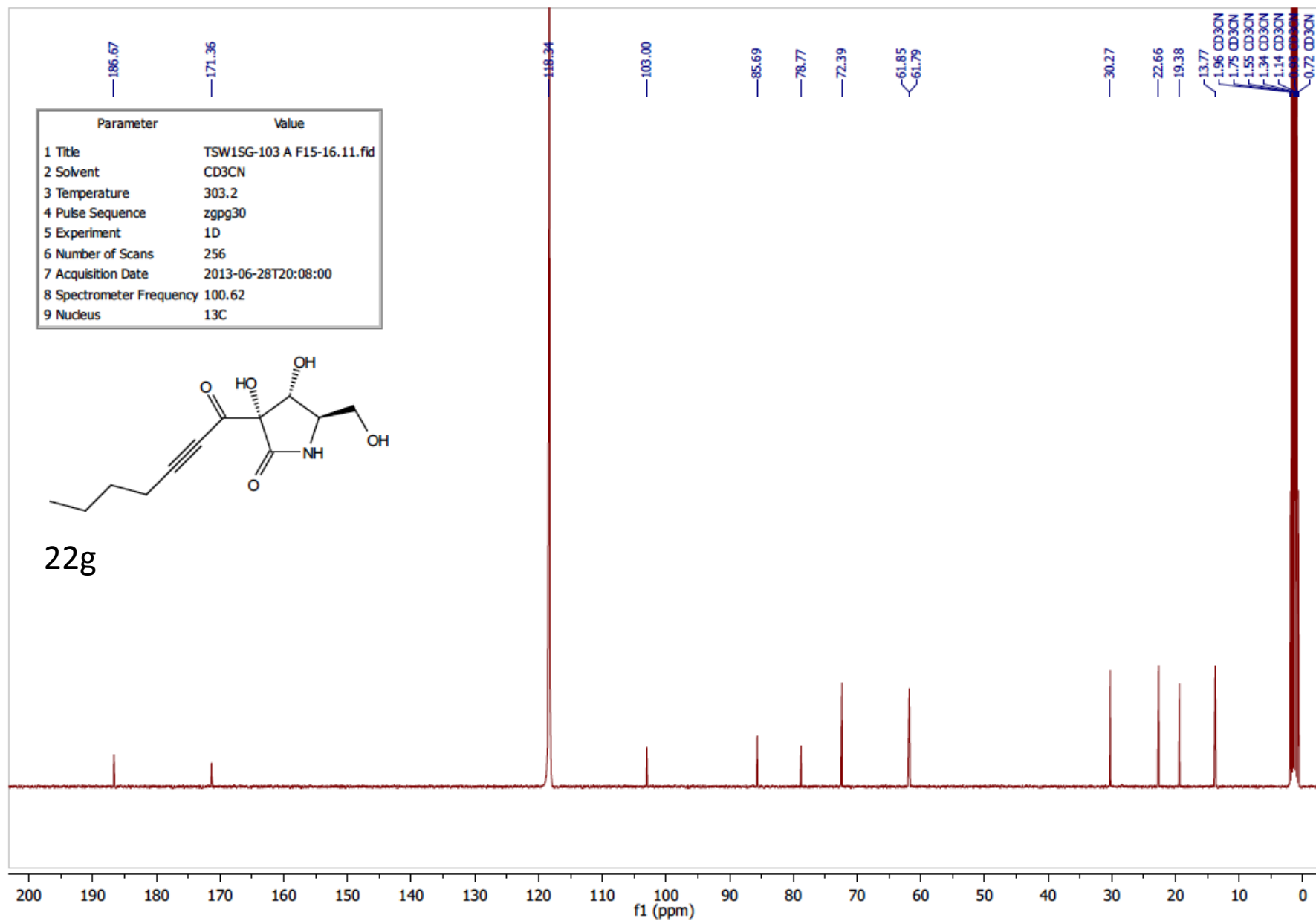


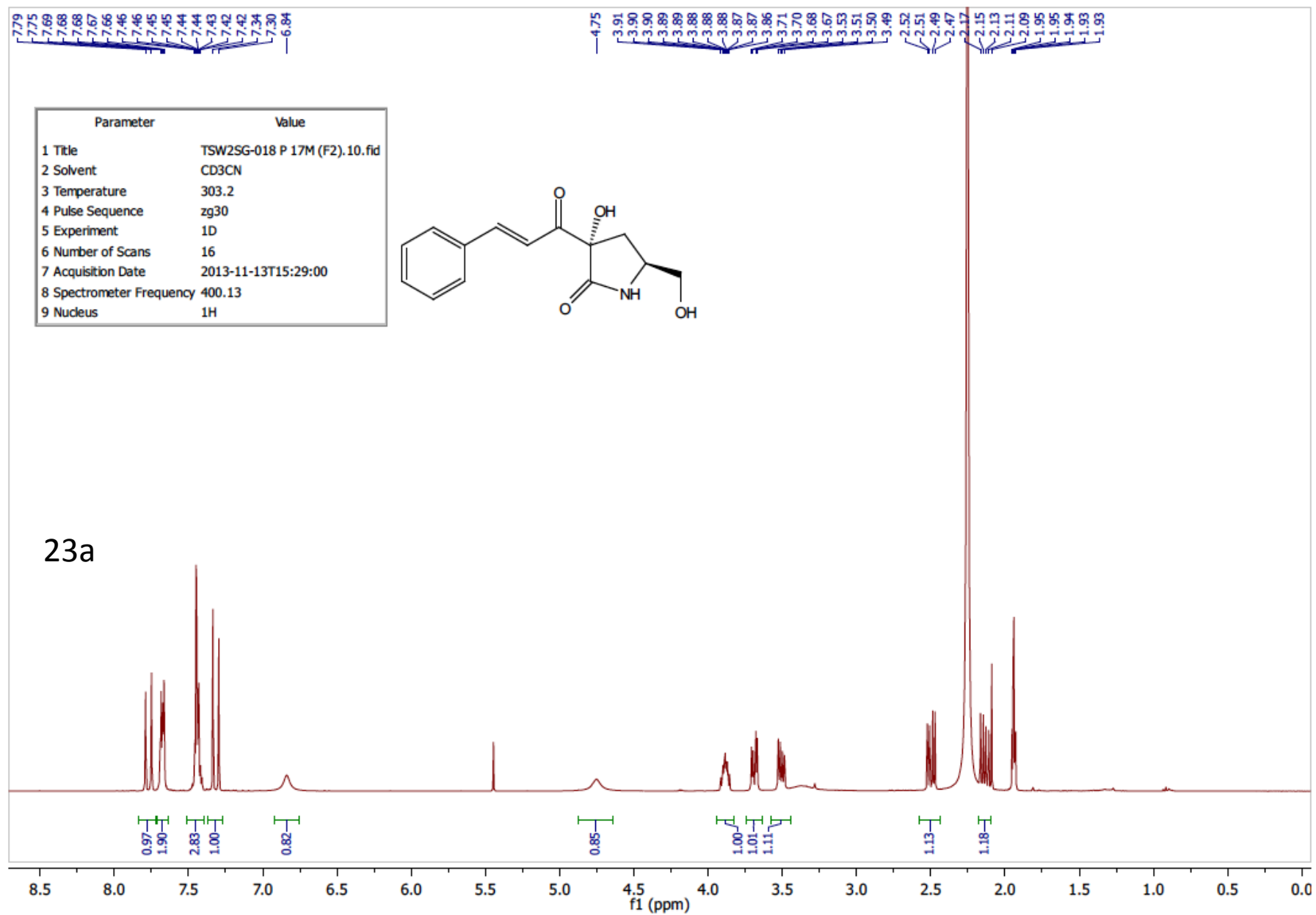


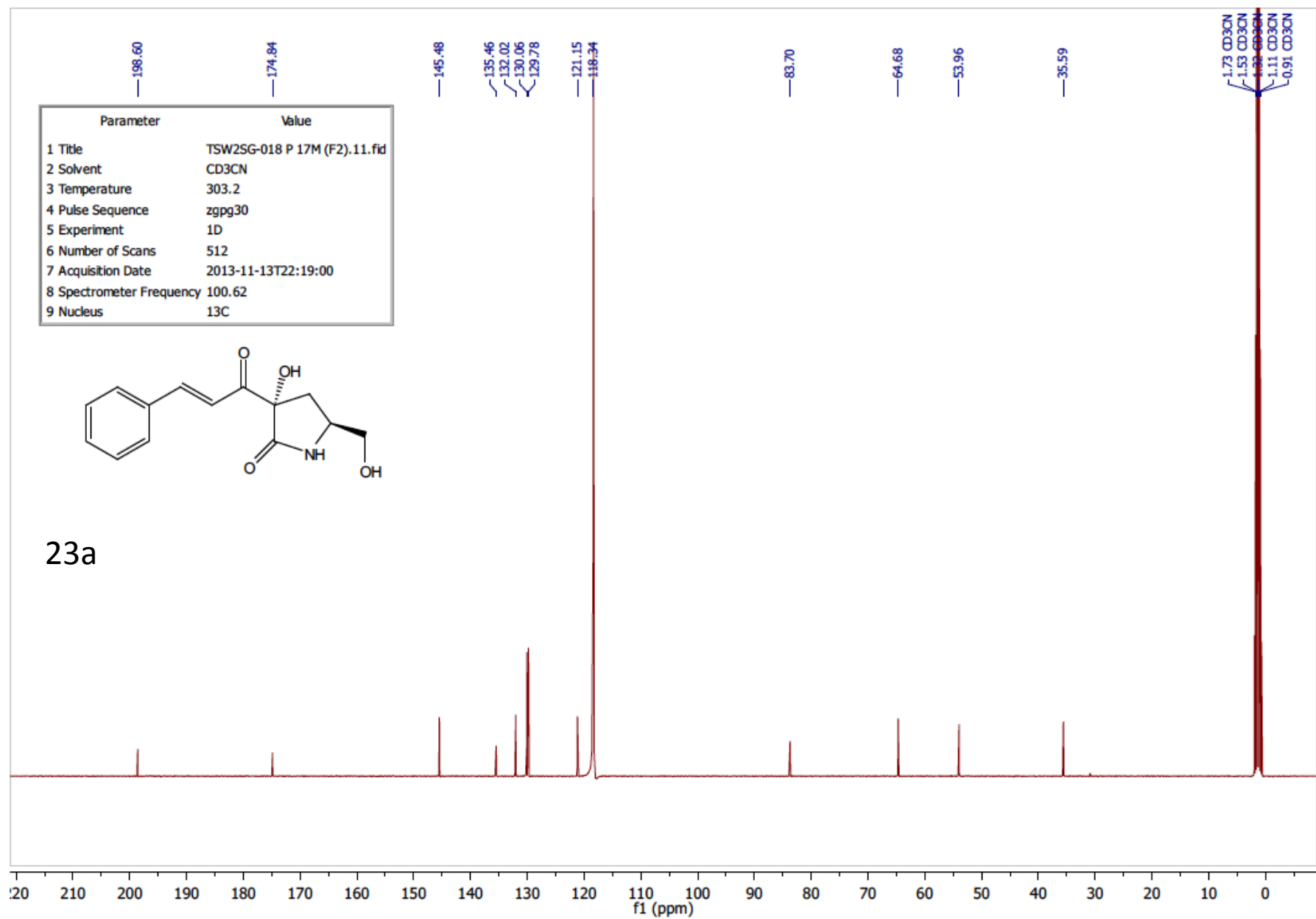


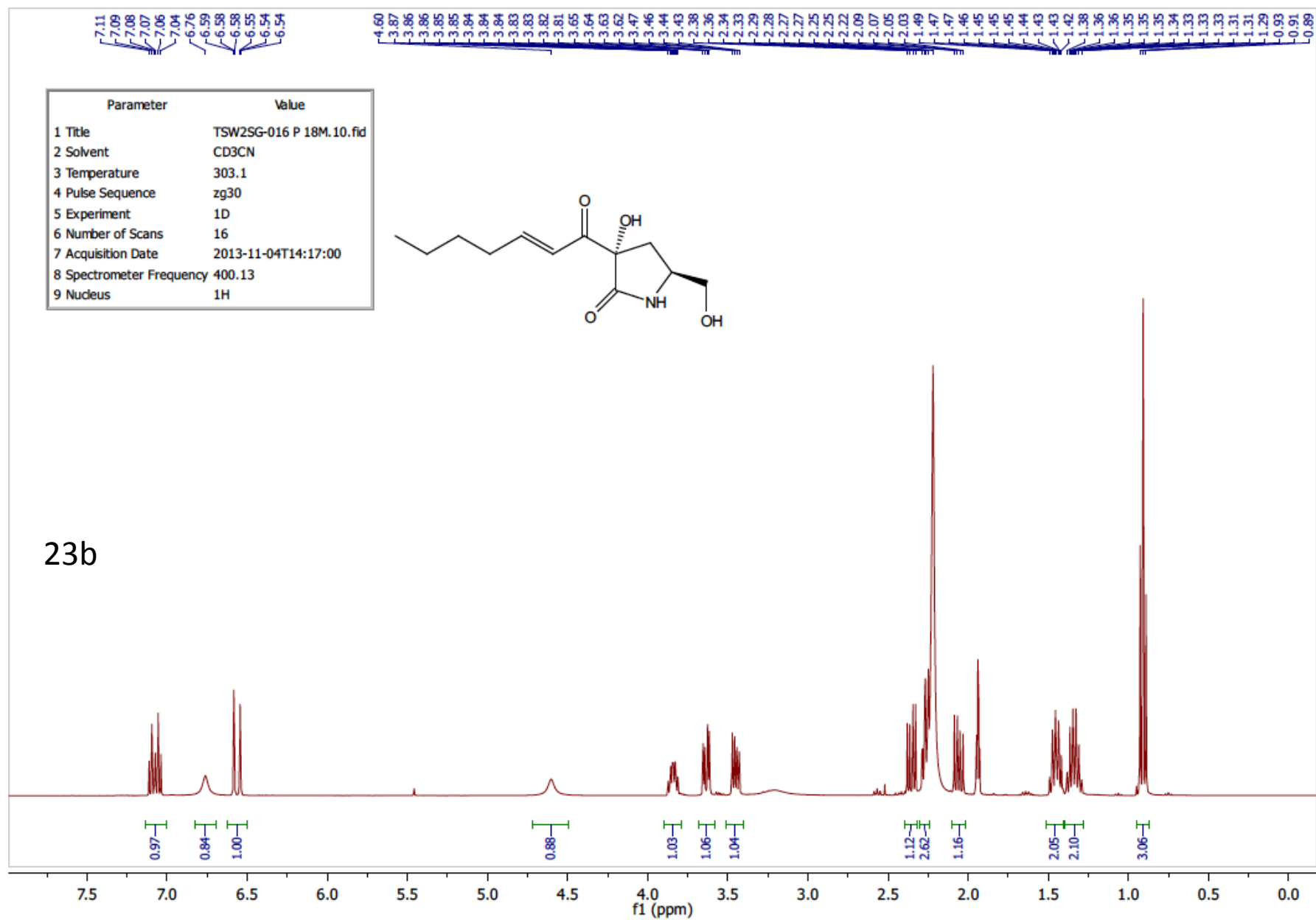


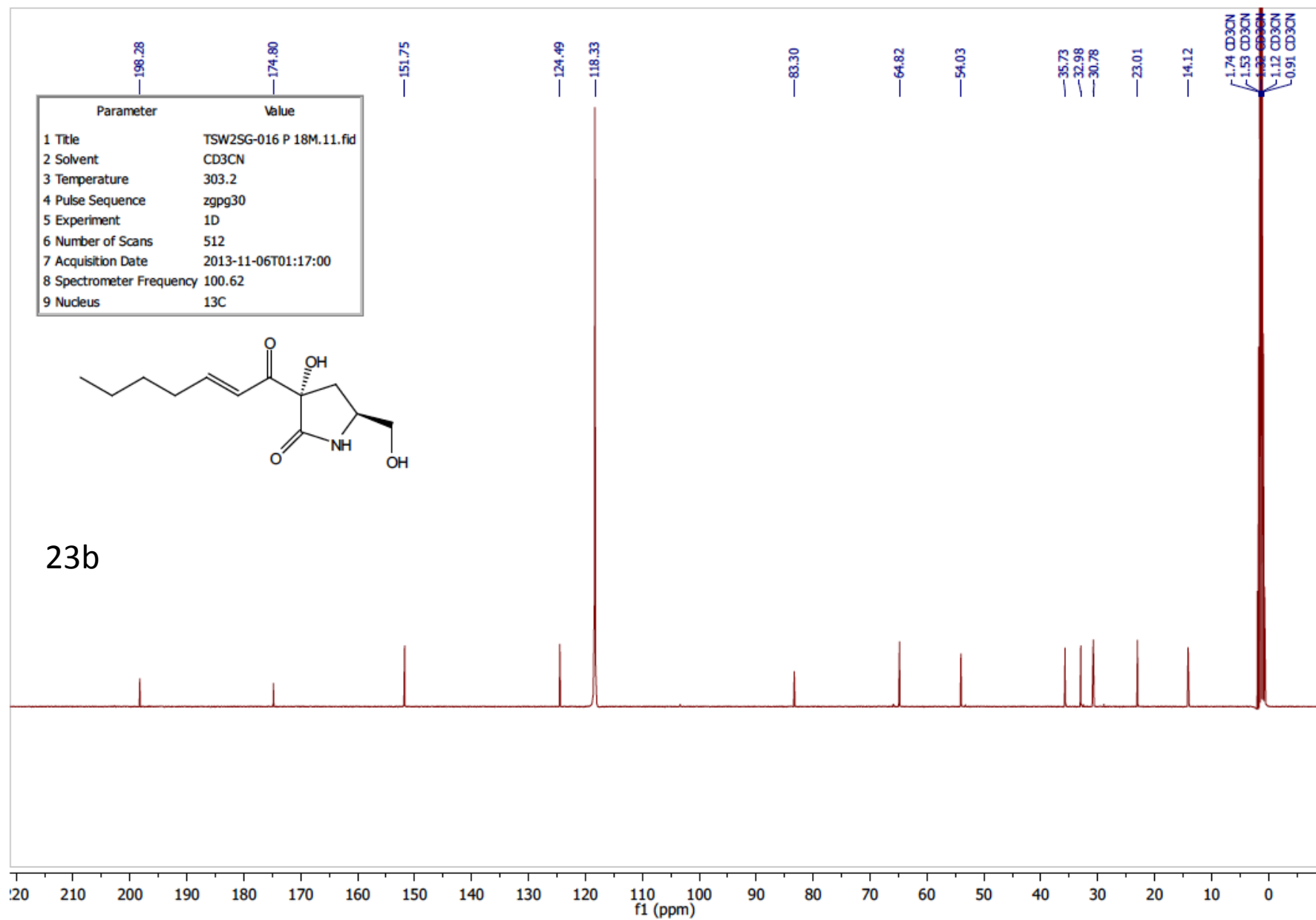


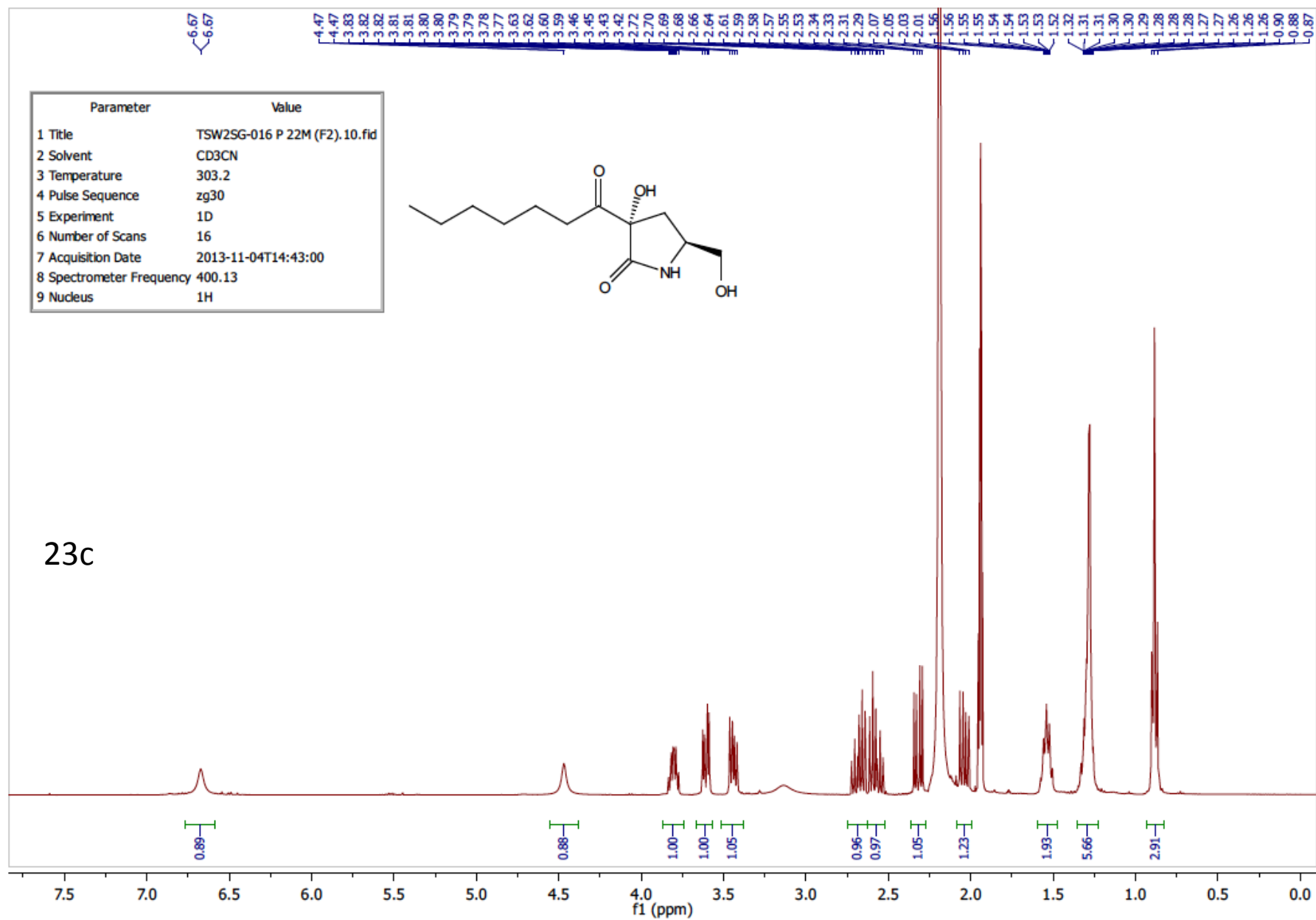


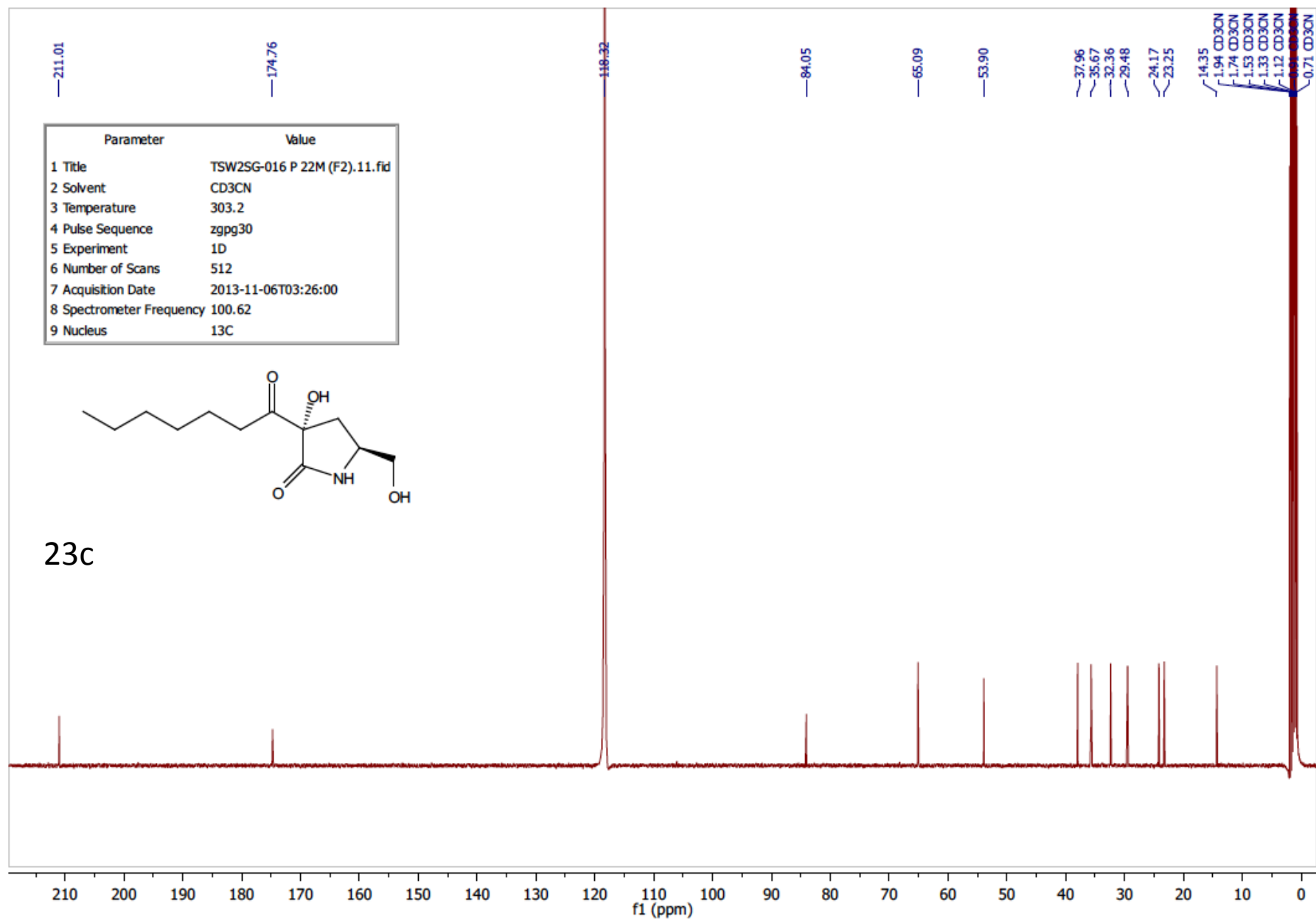


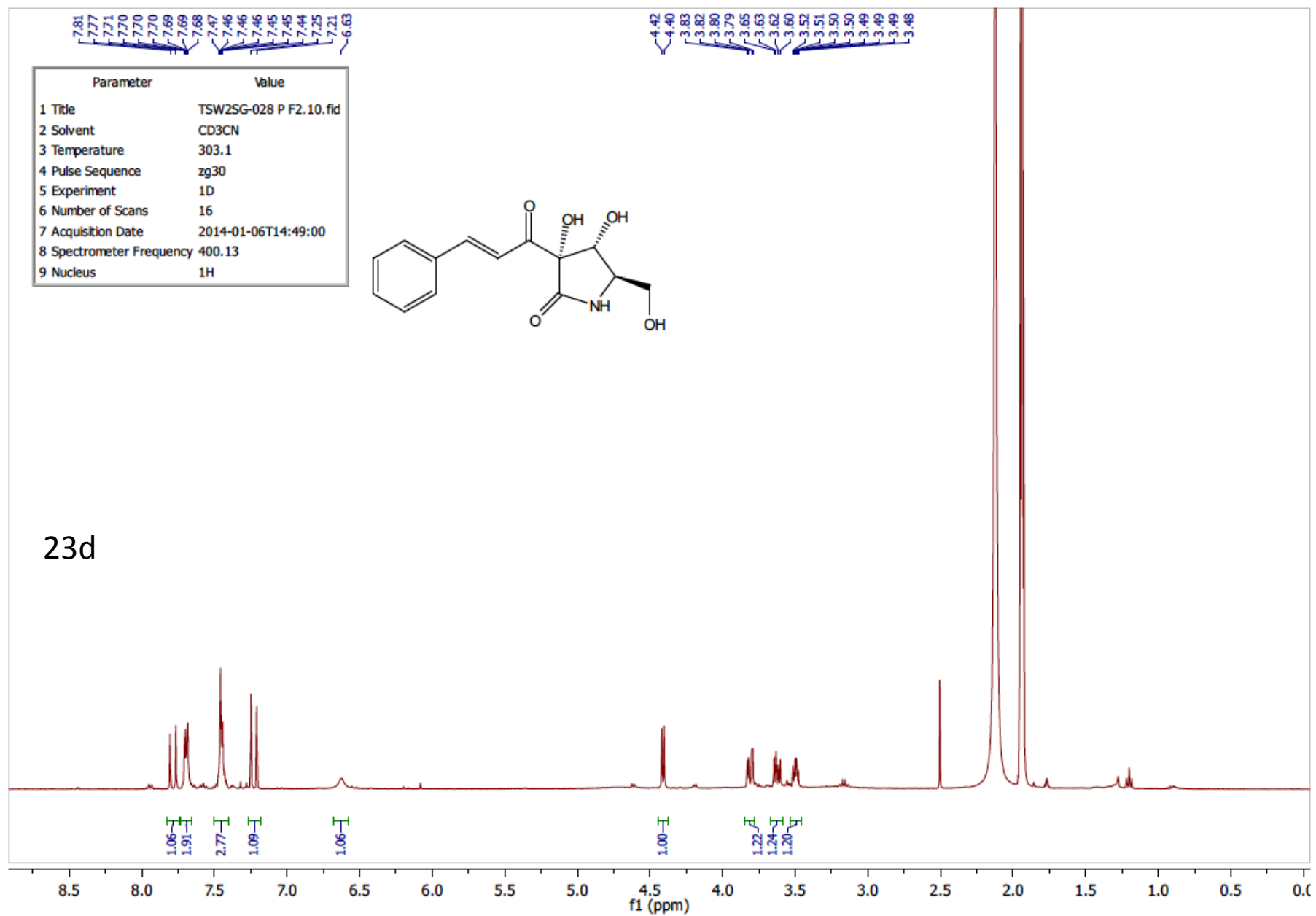


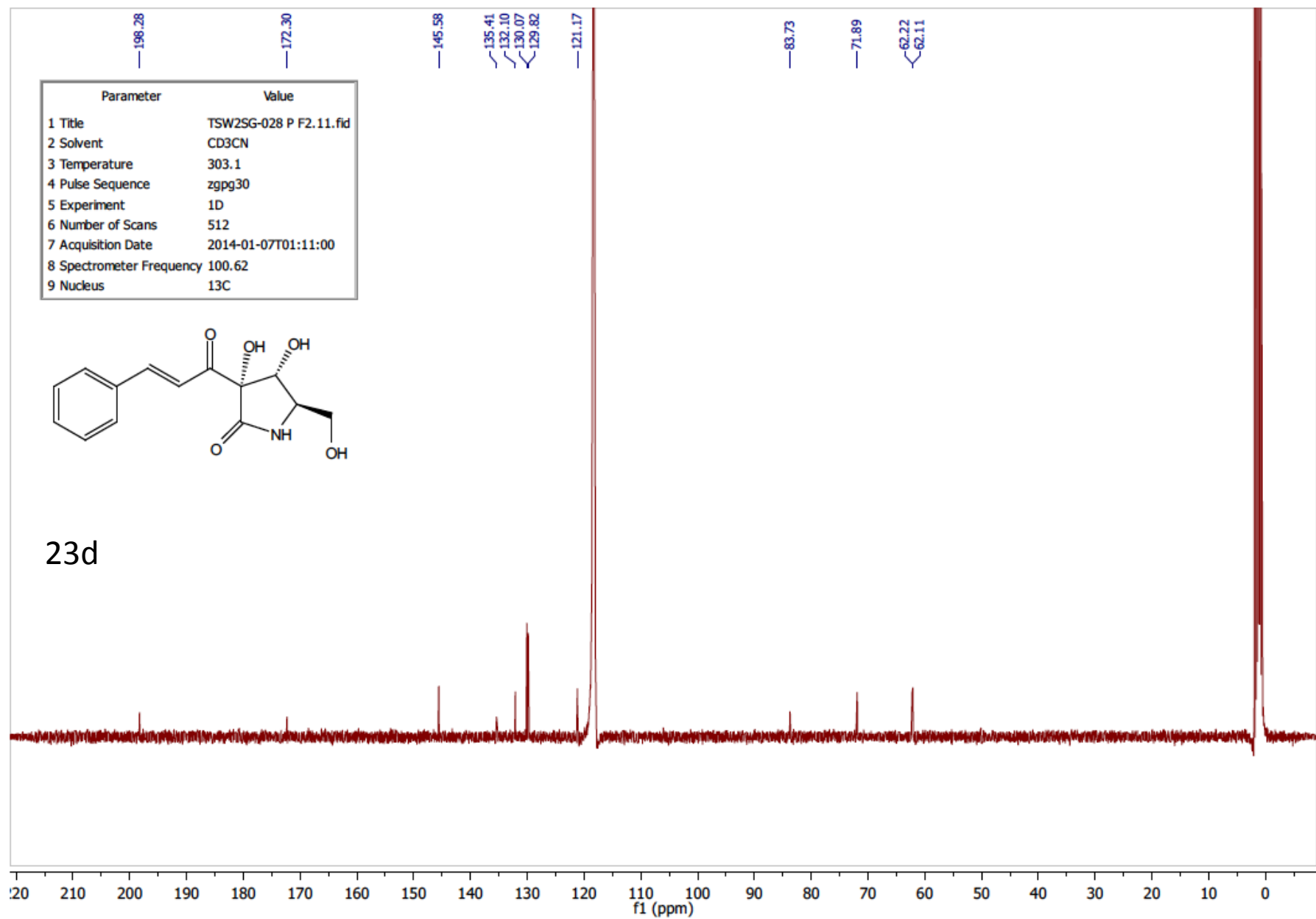


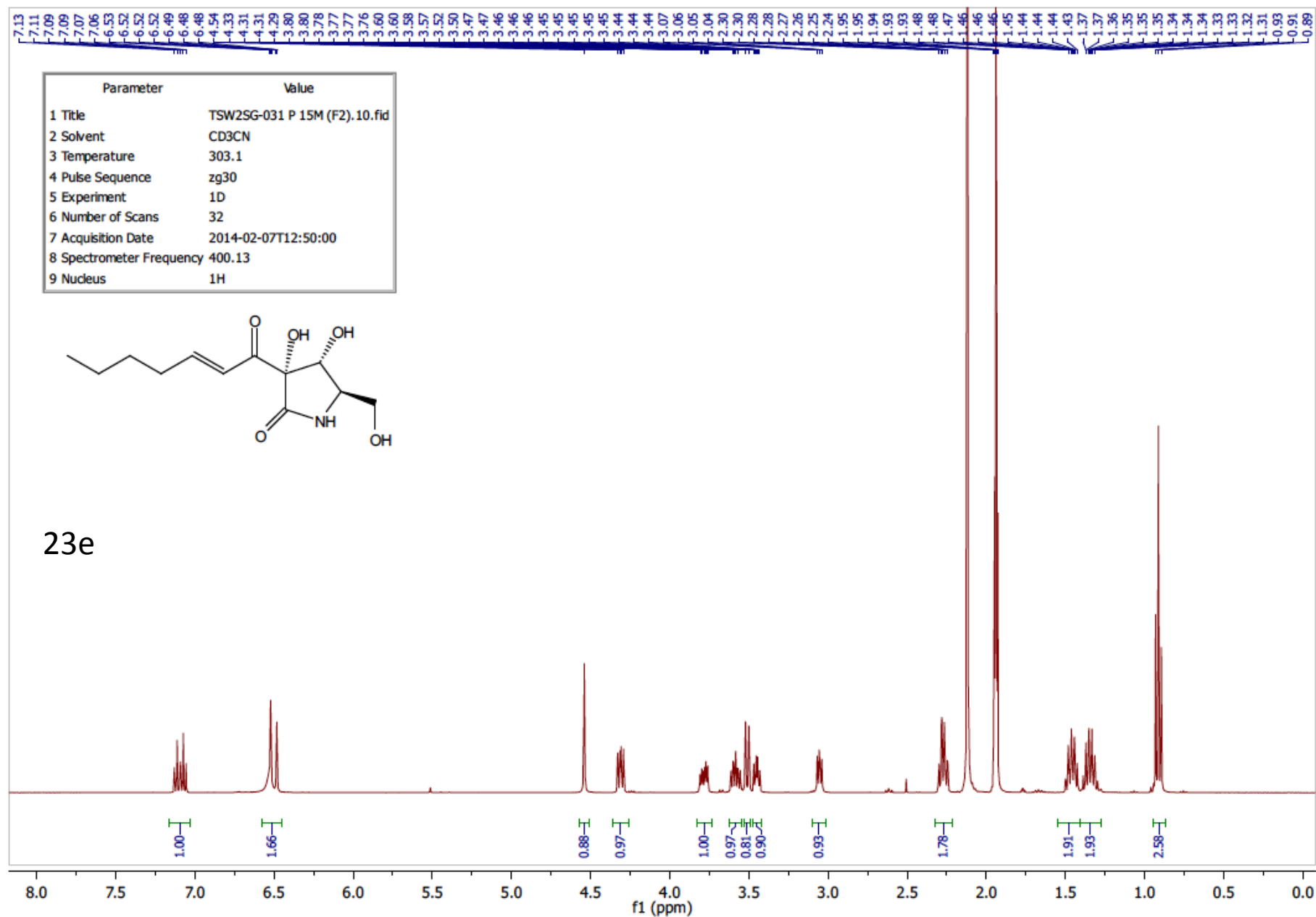


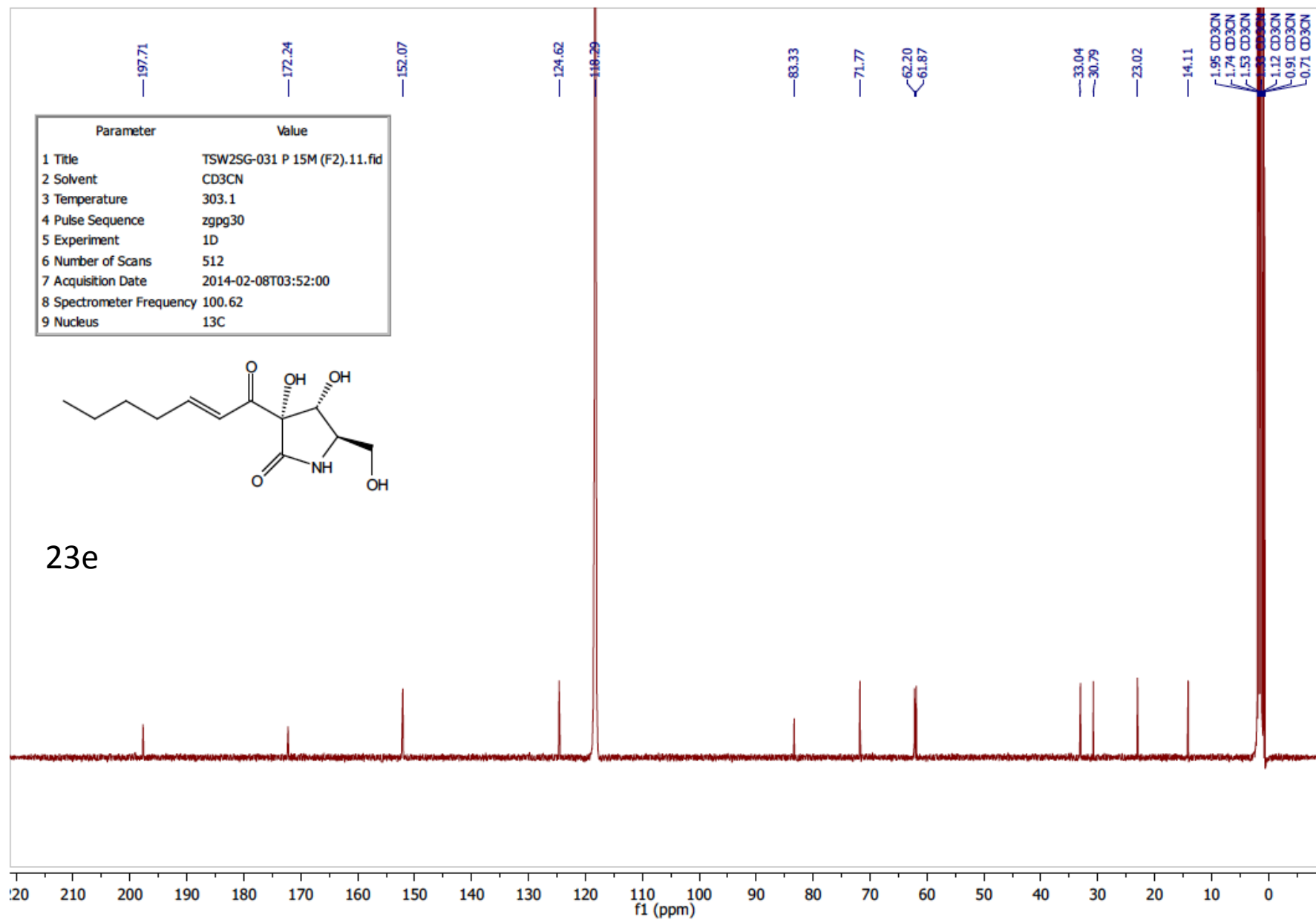


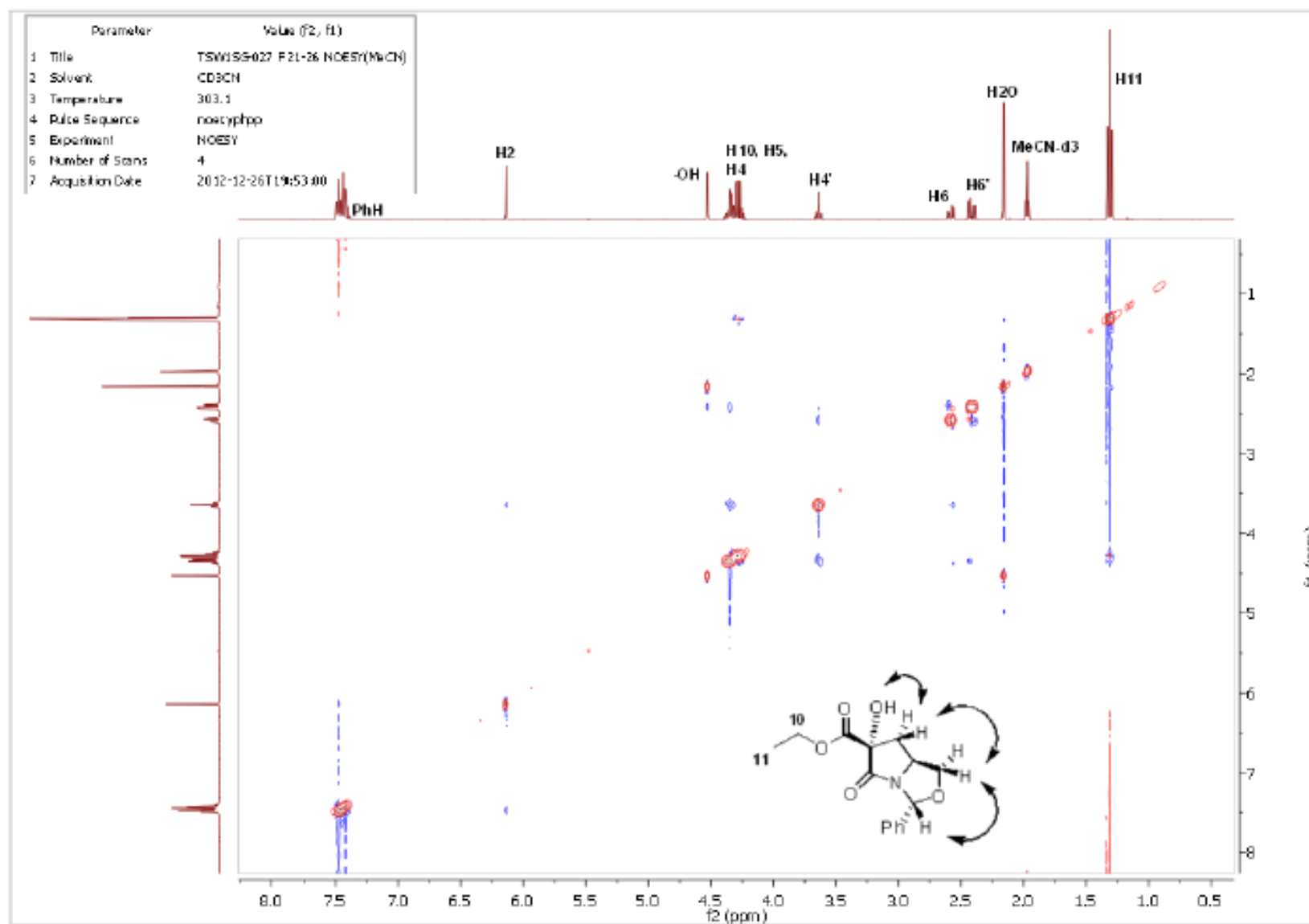
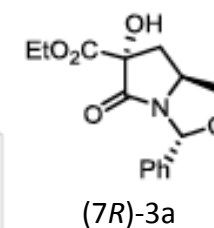


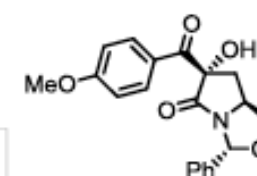




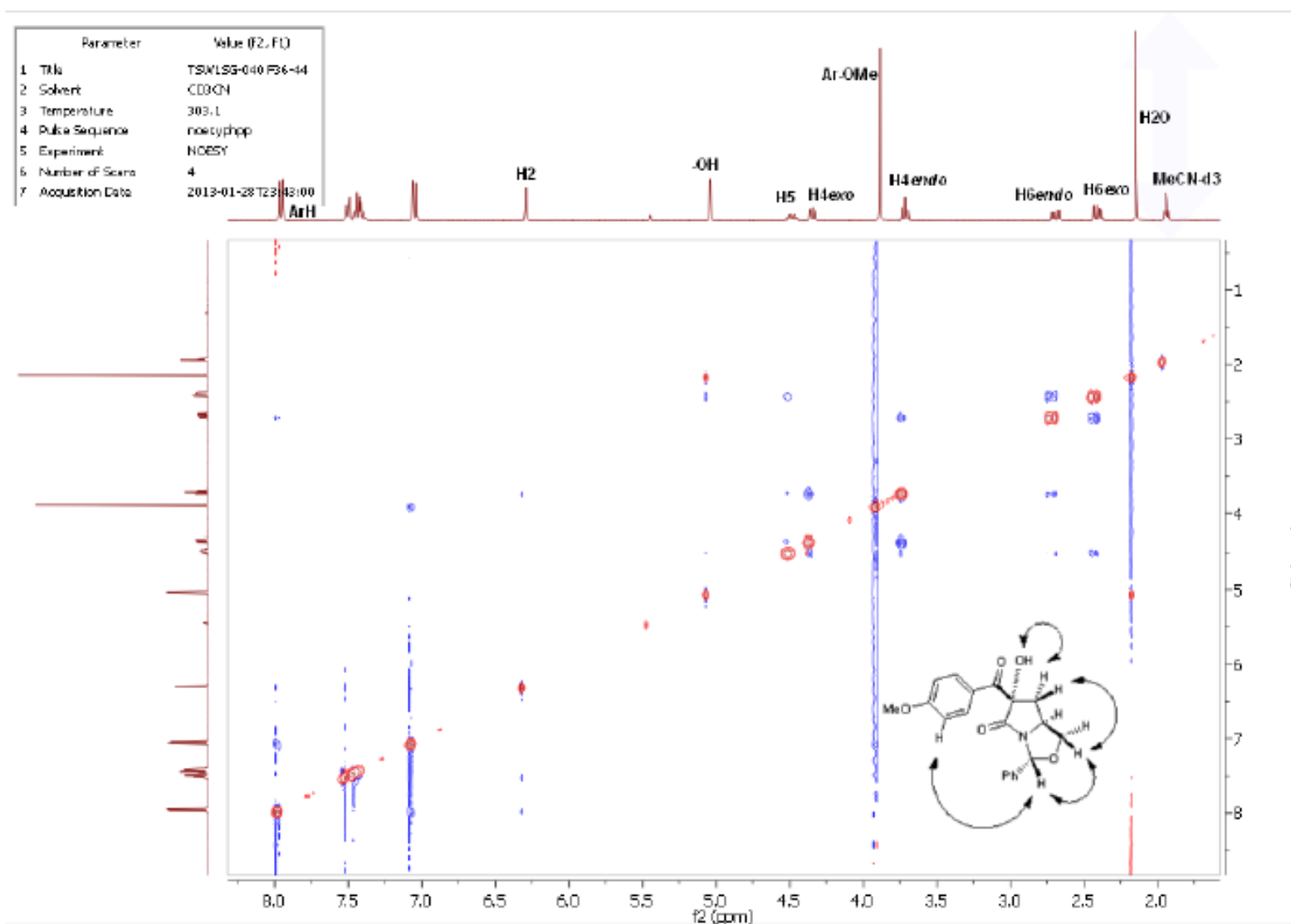


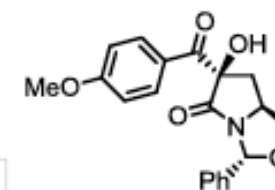




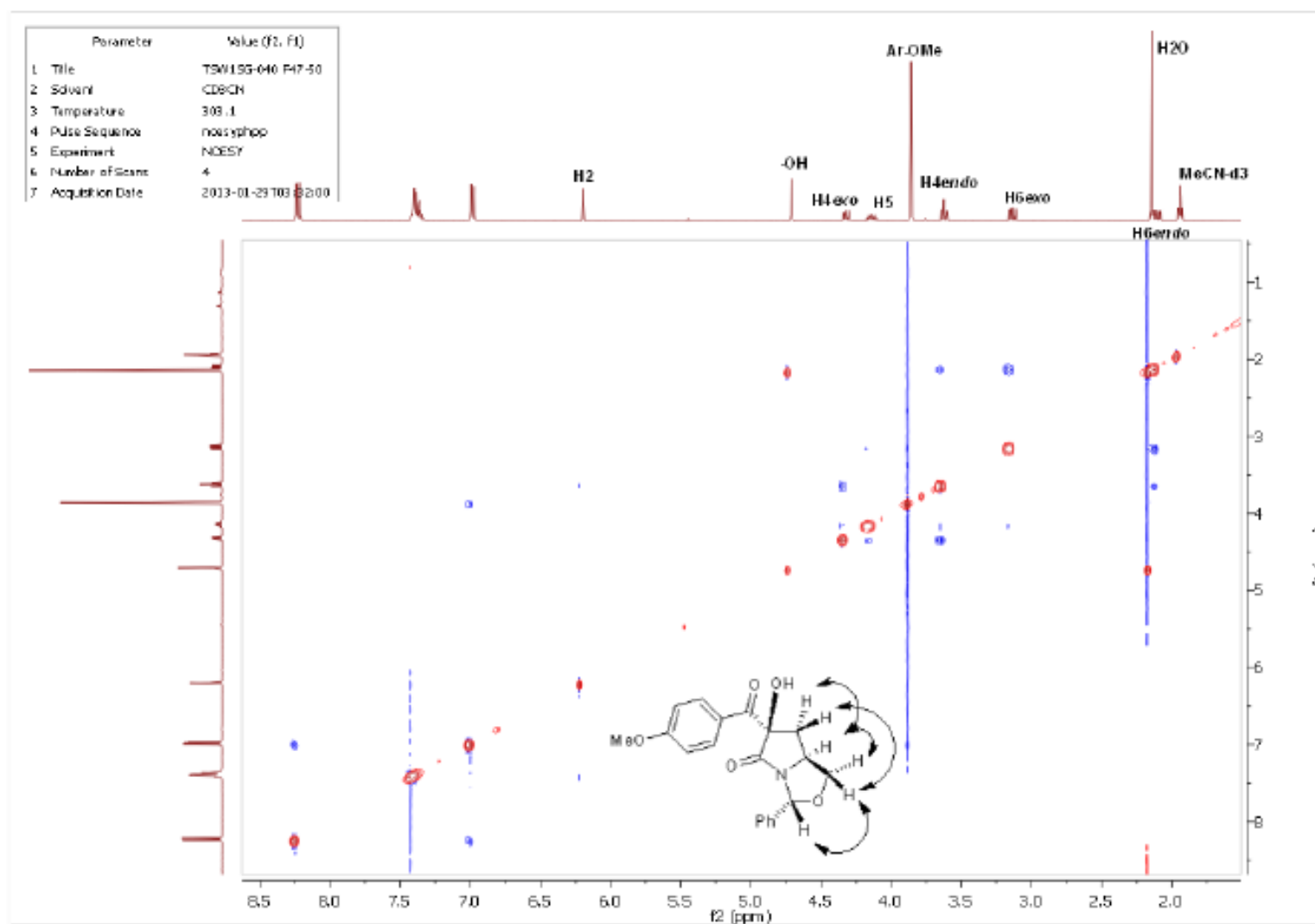


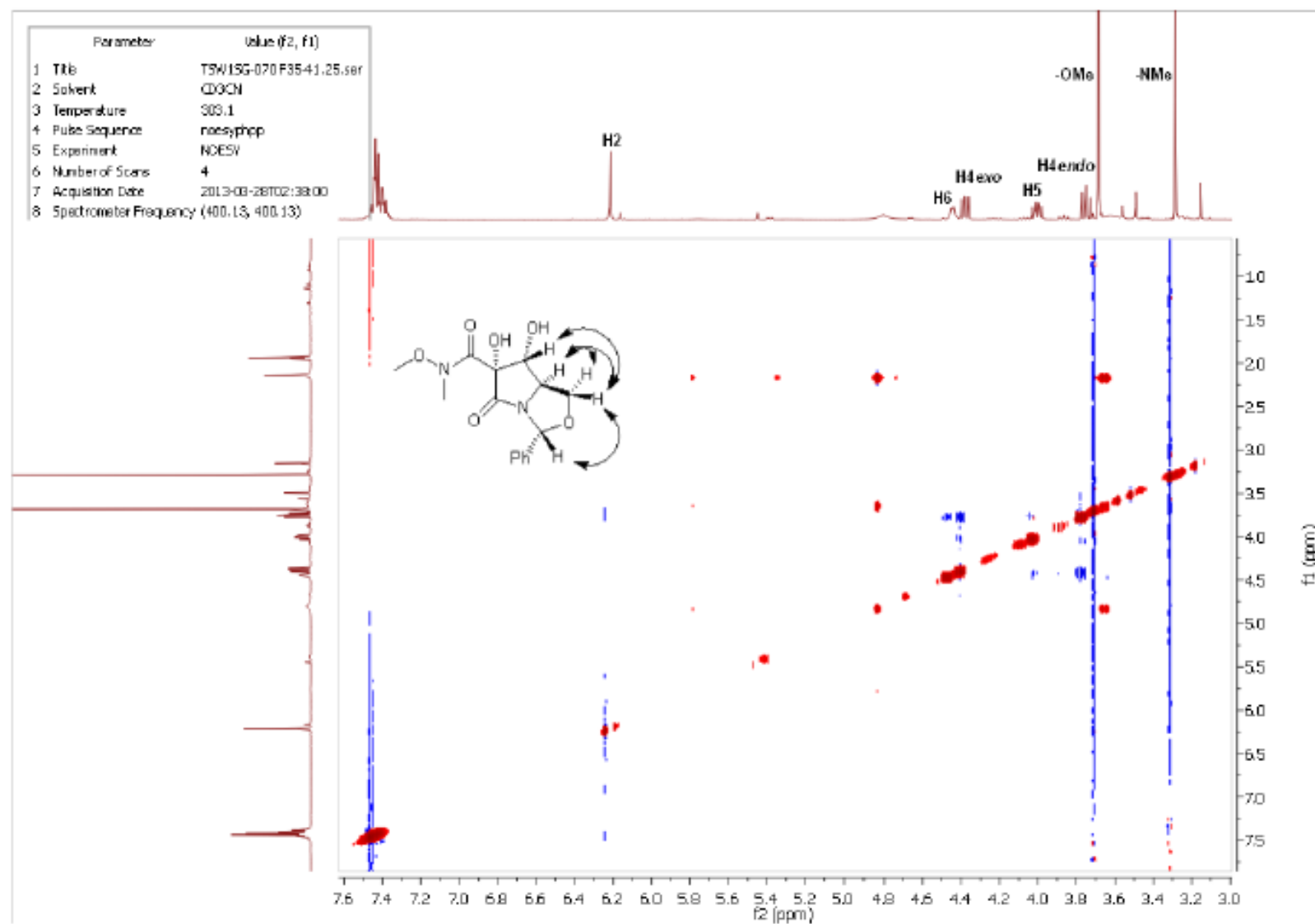
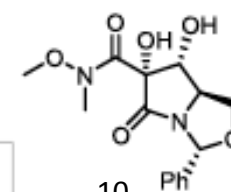
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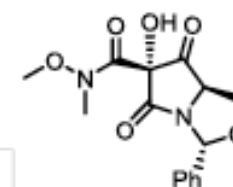




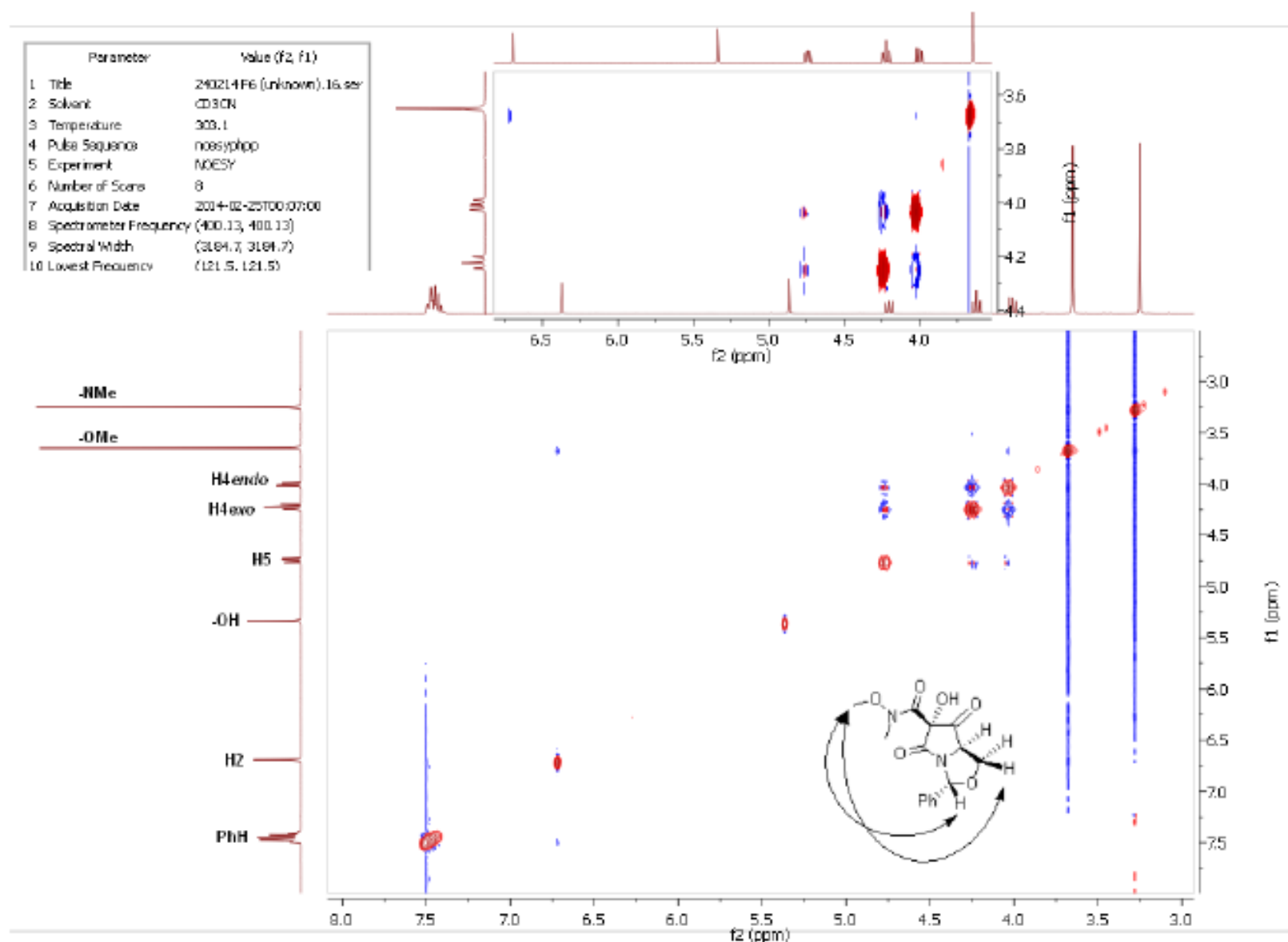
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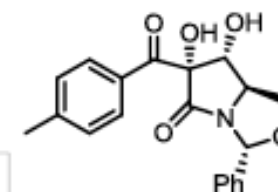




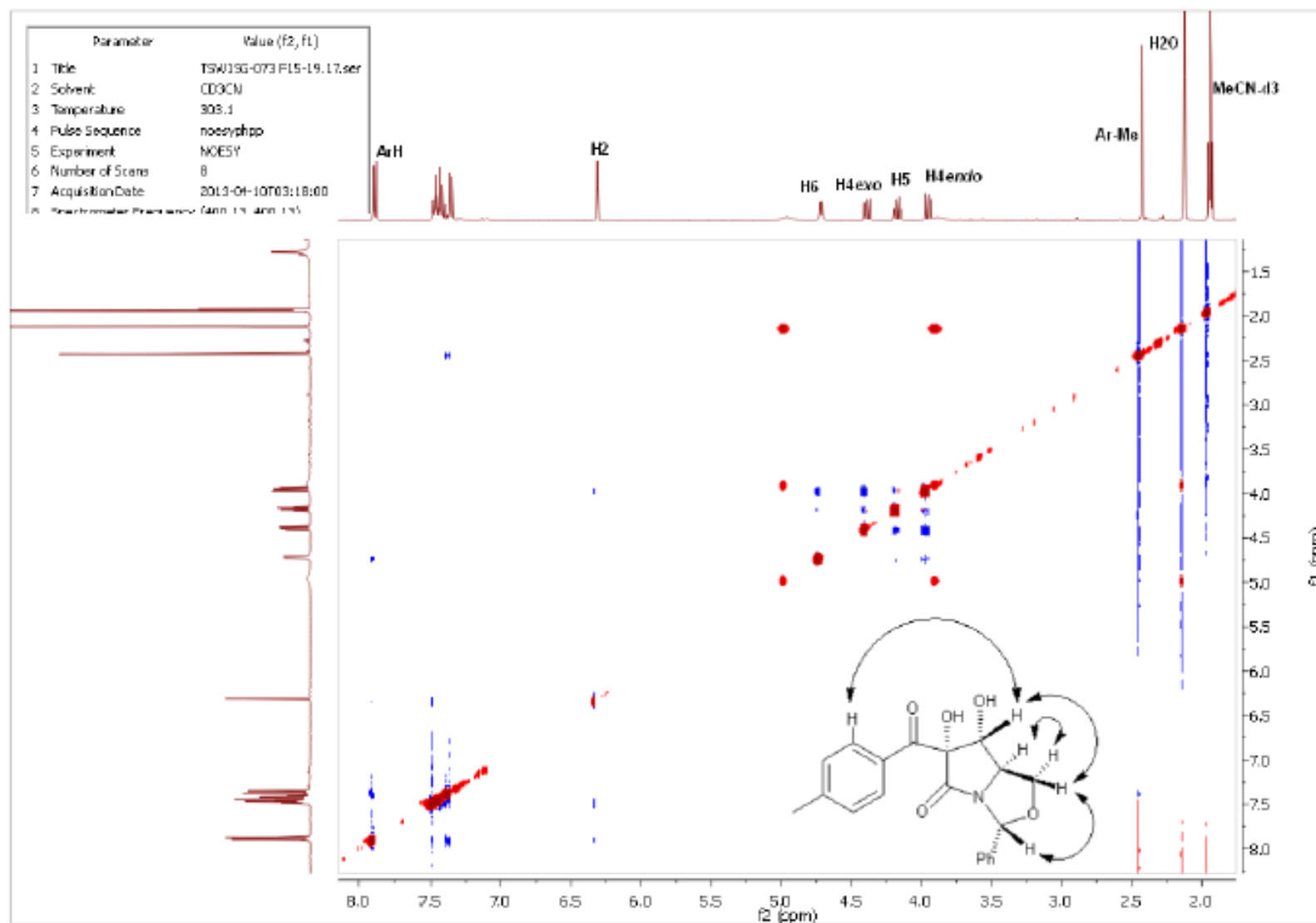


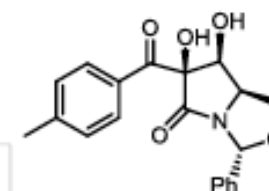
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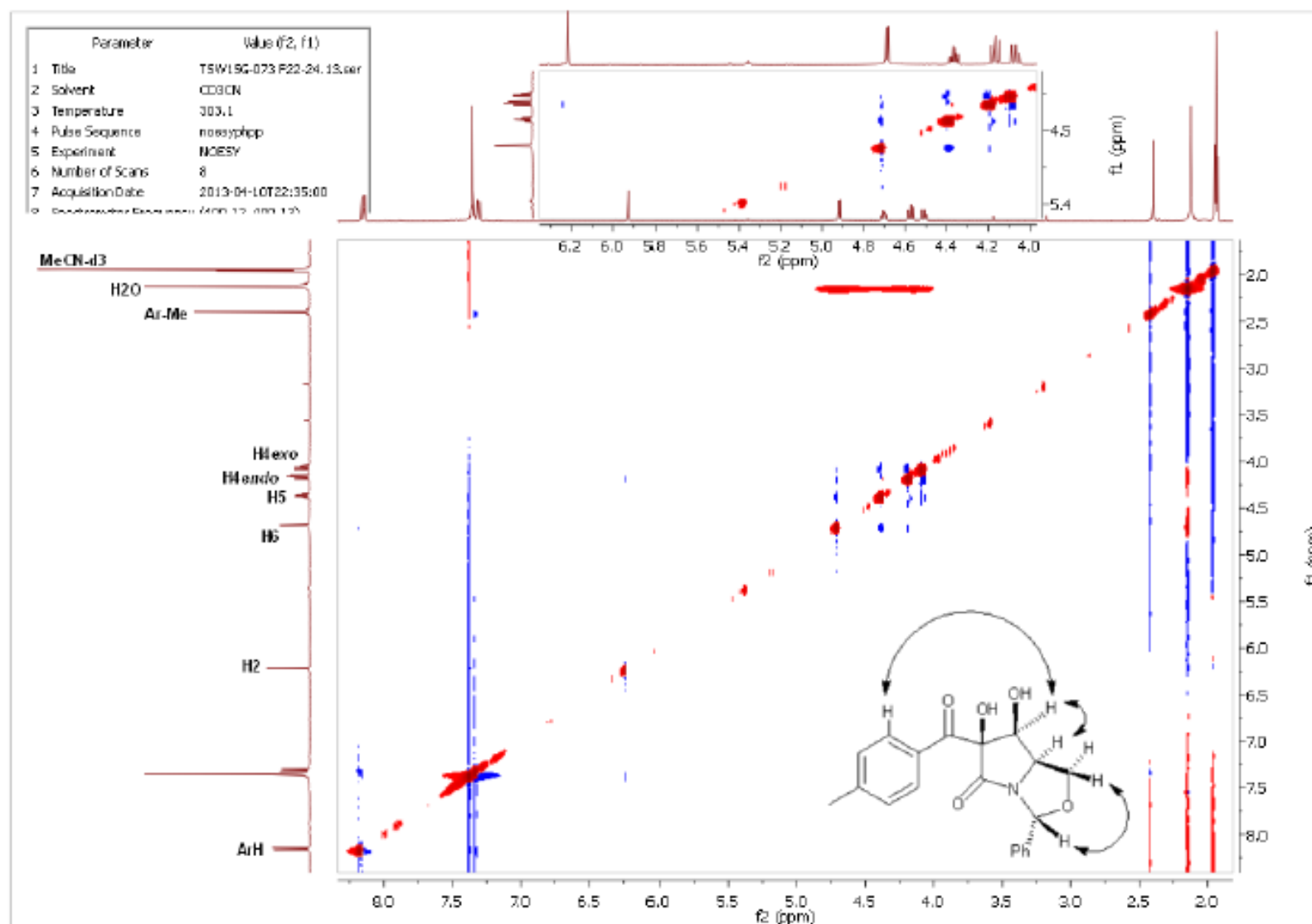


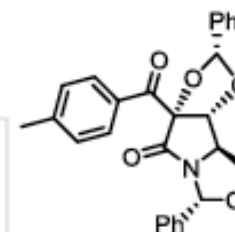
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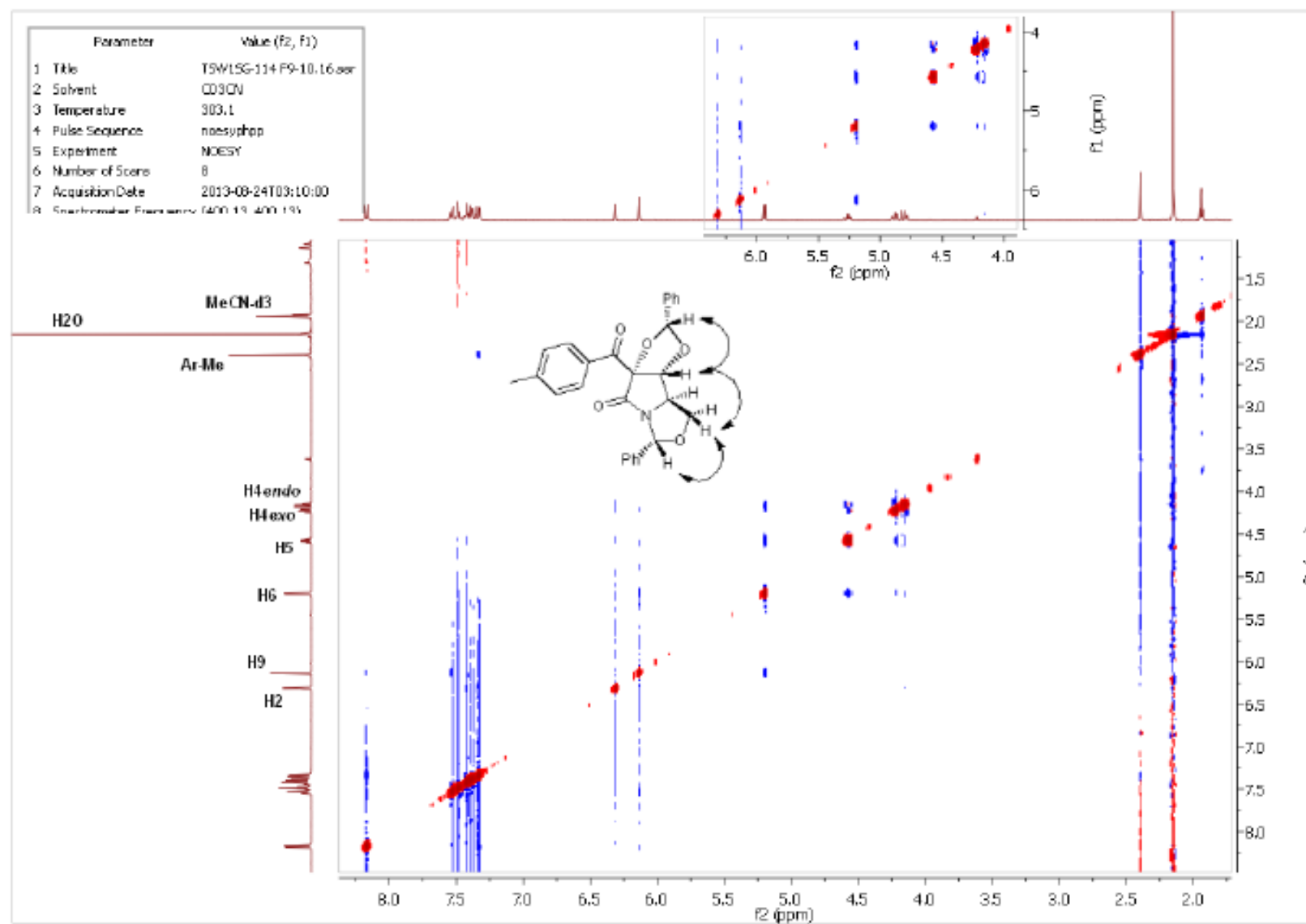


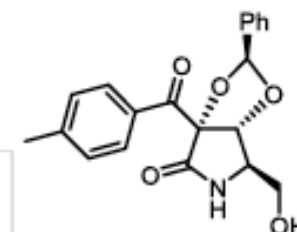
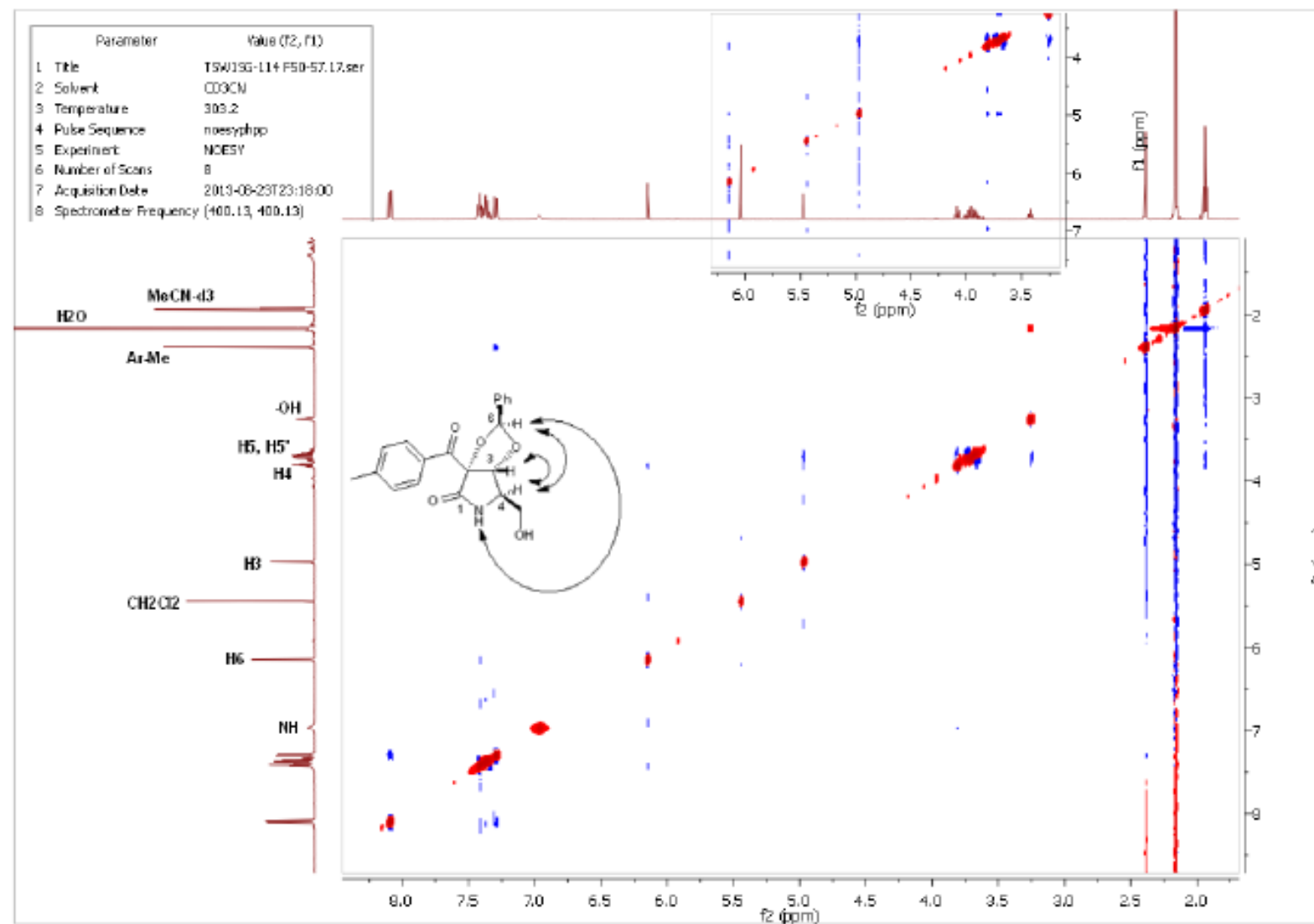
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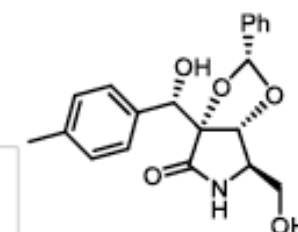
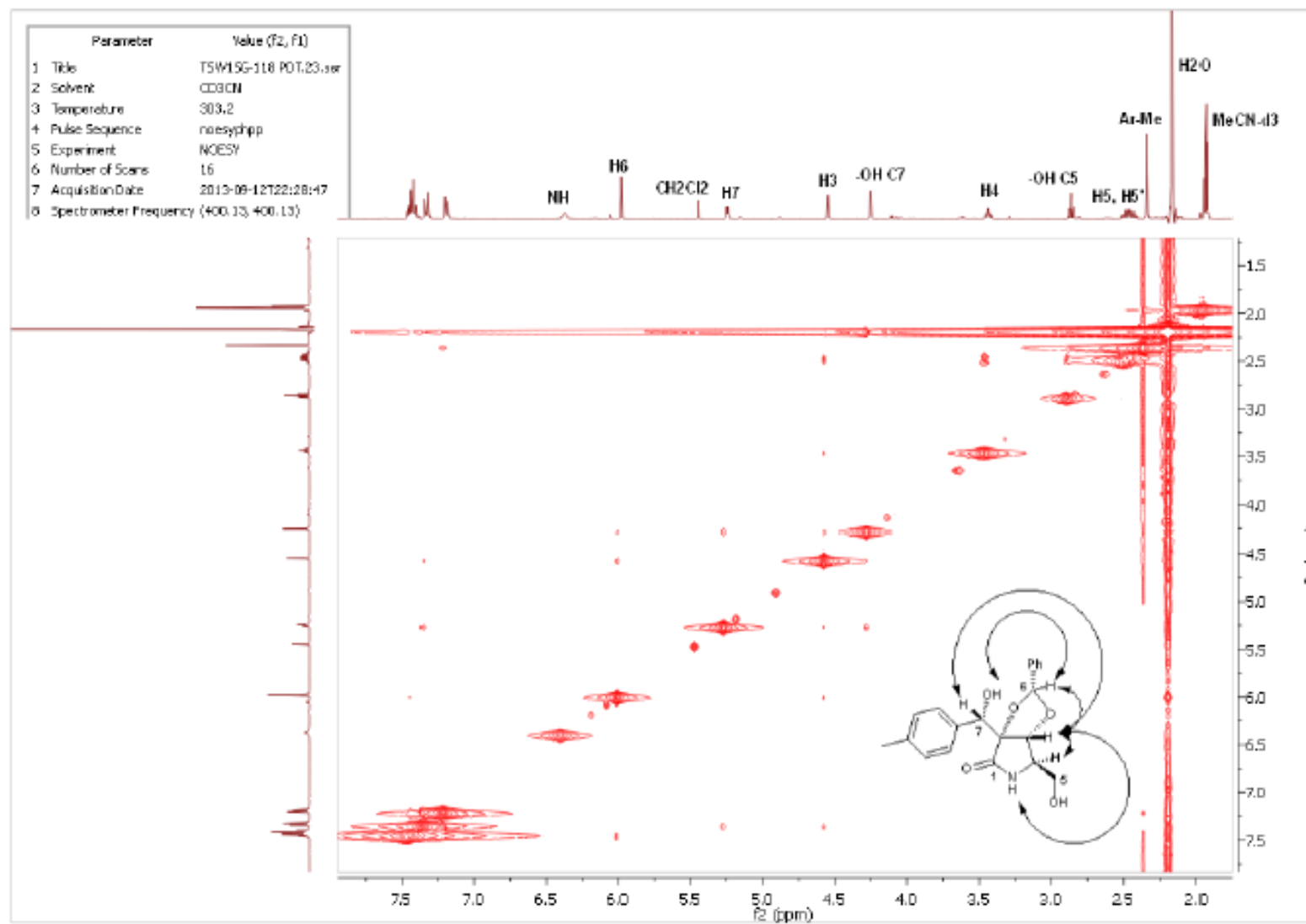


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## APPENDIX A: HOLE-PLATE ANTIBACTERIAL ASSAY

Agar plates for the bioassay were prepared by Wendy Sobey, and the testing for some of the compounds were carried out by Tharindi Panduwawala. Samples were tested on agar plates inoculated with *E. coli* X580 and *S. aureus* DS267 respectively. A 70% DMSO/H<sub>2</sub>O solution of each compound to be tested was prepared in concentrations of 4, 2, 1, 0.5 mg/mL via serial dilution of the most concentrated sample. A 100  $\mu$ L aliquot of each solution was loaded into a 10 mm well, and the plates were covered and incubated at 37°C between 16 and 20 h. The diameters of the resultant inhibition zones were then measured ( $\pm 0.5$  mm). A set of calibration data, using Cephalosporin C (CephC) as a standard, was also collected simultaneously with each run of bioassays.

### A.1 Calibration data for hole-plate antibacterial assay

An example of a calibration data set is illustrated below with the respective calibration curves.

Table A.1: An example of calibration data for one of the bioassays.

| Conc. of stock soln. ( $\mu$ g/mL) | Vol. of CephC stock ( $\mu$ L/well) | Vol. of water ( $\mu$ L/well) | Mass of CephC ( $\mu$ g/well) | Moles of CephC (nmol/well) | Zone size (mm) | Log (nmol CephC) |
|------------------------------------|-------------------------------------|-------------------------------|-------------------------------|----------------------------|----------------|------------------|
| <i>S. aureus</i>                   |                                     |                               |                               |                            |                |                  |
| 1000                               | 20                                  | 80                            | 20                            | 48.14                      | Not active     | 1.683            |
|                                    | 40                                  | 60                            | 40                            | 96.29                      | 13.5           | 1.984            |
|                                    | 60                                  | 40                            | 60                            | 144.44                     | 16.0           | 2.160            |
|                                    | 80                                  | 20                            | 80                            | 192.59                     | 19.0           | 2.285            |
|                                    | 100                                 | 0                             | 100                           | 240.73                     | 21.0           | 2.382            |
| <i>E. coli</i>                     |                                     |                               |                               |                            |                |                  |
| 10                                 | 20                                  | 80                            | 0.2                           | 0.4815                     | Not active     | -0.3174          |
|                                    | 40                                  | 60                            | 0.4                           | 0.9629                     | 19             | -0.0164          |
|                                    | 60                                  | 40                            | 0.6                           | 1.4444                     | 22             | 0.1597           |
|                                    | 80                                  | 20                            | 0.8                           | 1.9259                     | 25             | 0.2846           |
|                                    | 100                                 | 0                             | 1                             | 2.4073                     | 30             | 0.3815           |
| 100                                | 20                                  | 80                            | 2                             | 4.8146                     | 31             | 0.6826           |
|                                    | 40                                  | 60                            | 4                             | 9.6293                     | 36             | 0.9836           |
|                                    | 60                                  | 40                            | 6                             | 12.4439                    | 38             | 1.1597           |
|                                    | 80                                  | 20                            | 8                             | 19.2585                    | 42             | 1.2846           |
|                                    | 100                                 | 0                             | 10                            | 24.0732                    | 44             | 1.3815           |

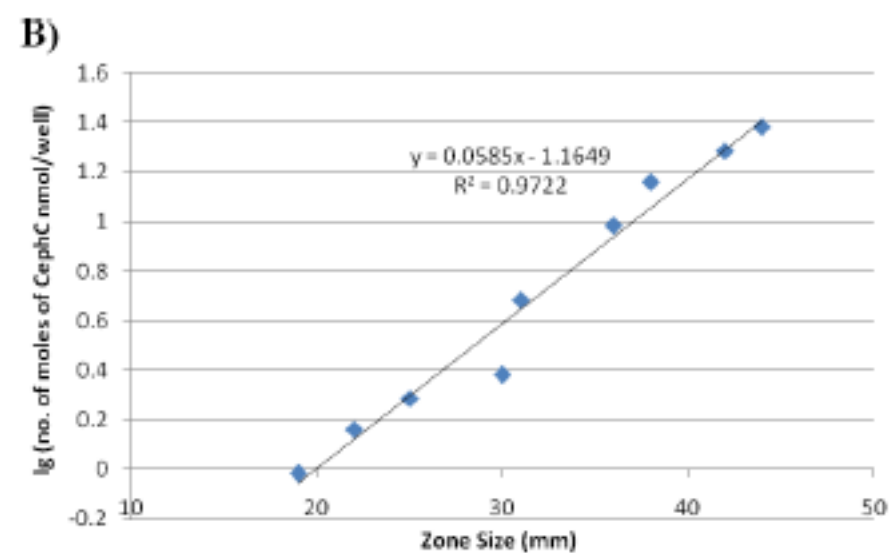
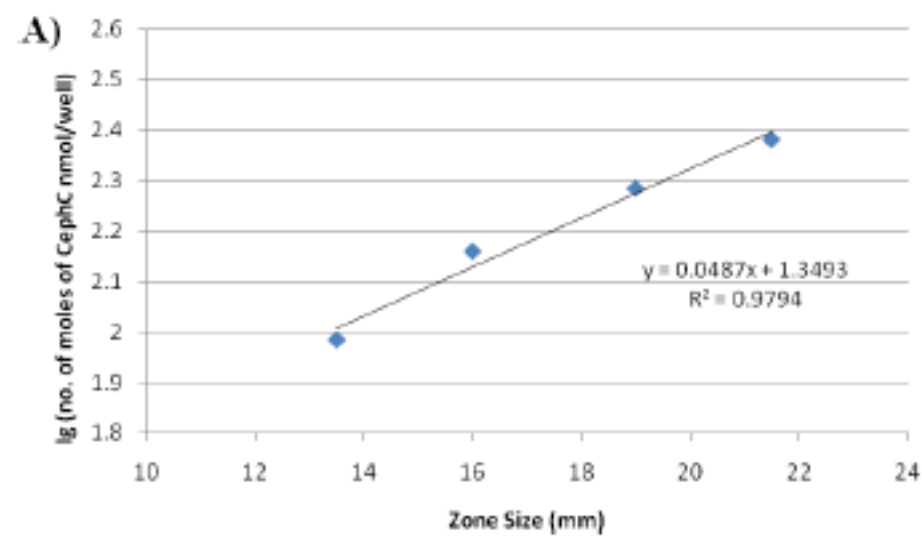
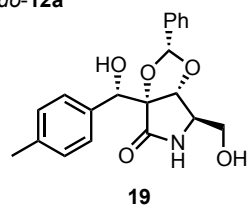
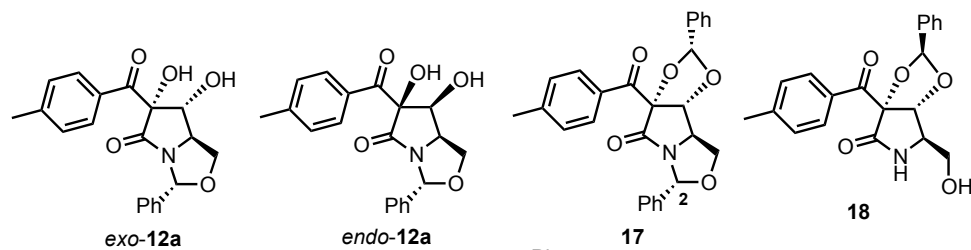
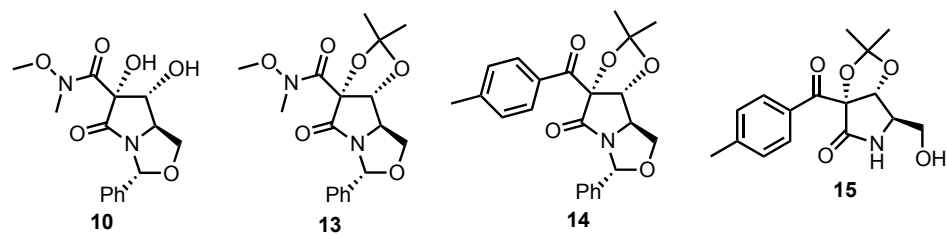
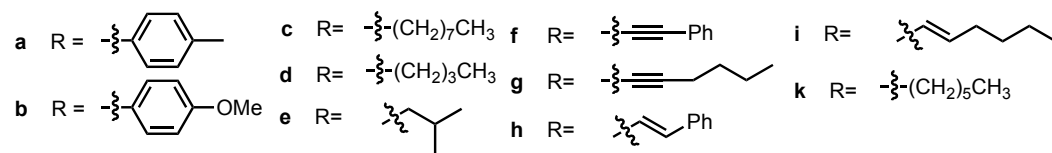
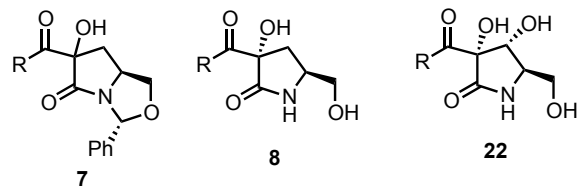
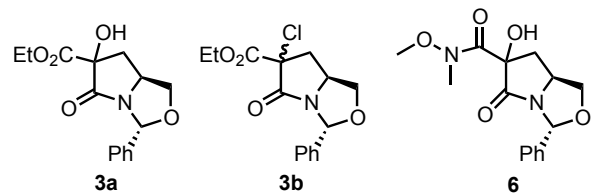


Figure A.1. Calibration curve for A) *S. aureus*; B) *E. coli*.



Figure