

## *Supporting Information*

### **STRUCTURE–ACTIVITY RELATIONSHIP STUDY OF GATASTATIN BASED ON THE TOPLISS TREE APPROACH**

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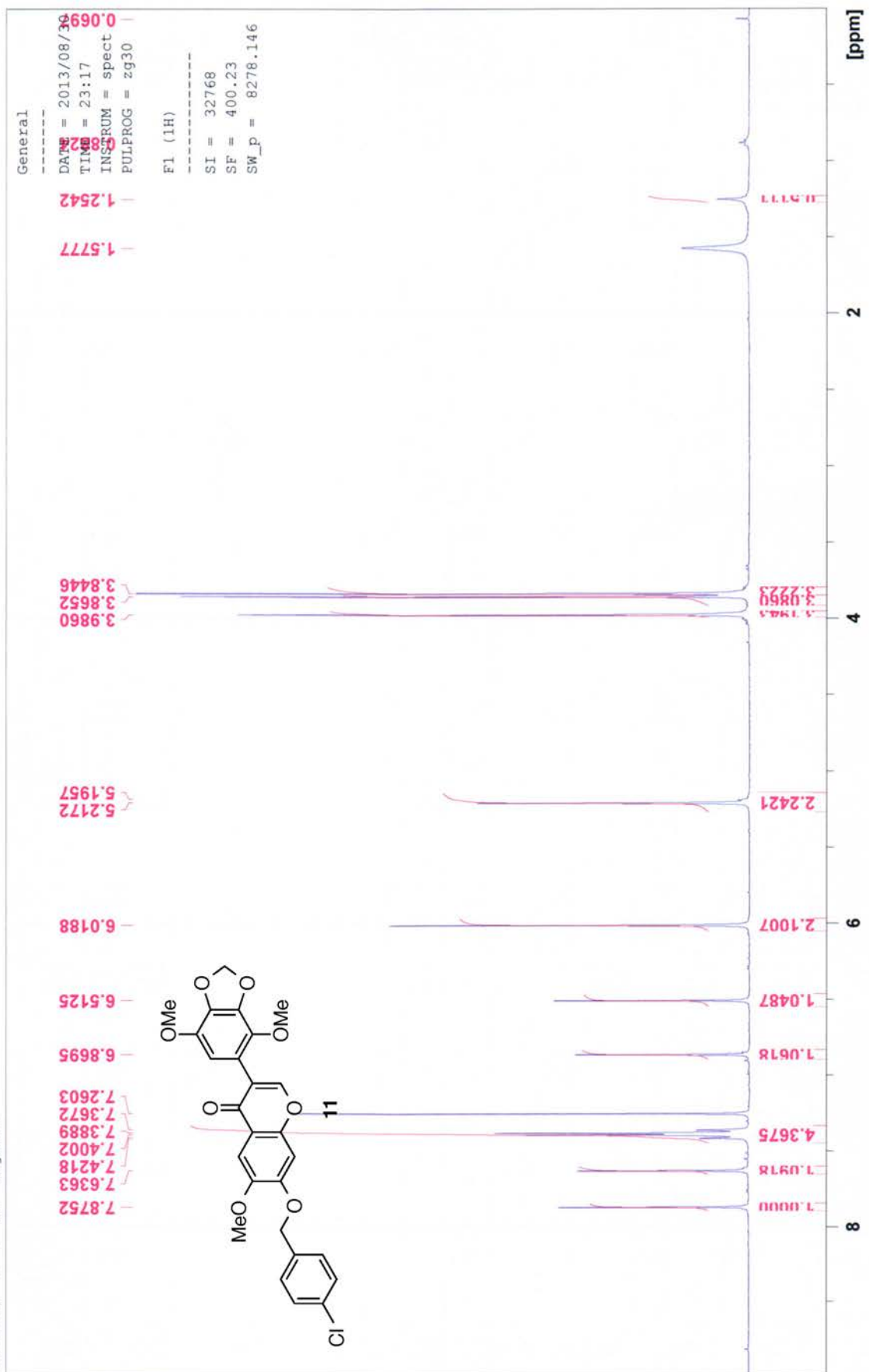
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<sup>1</sup>H and <sup>13</sup>C NMR spectra of compounds

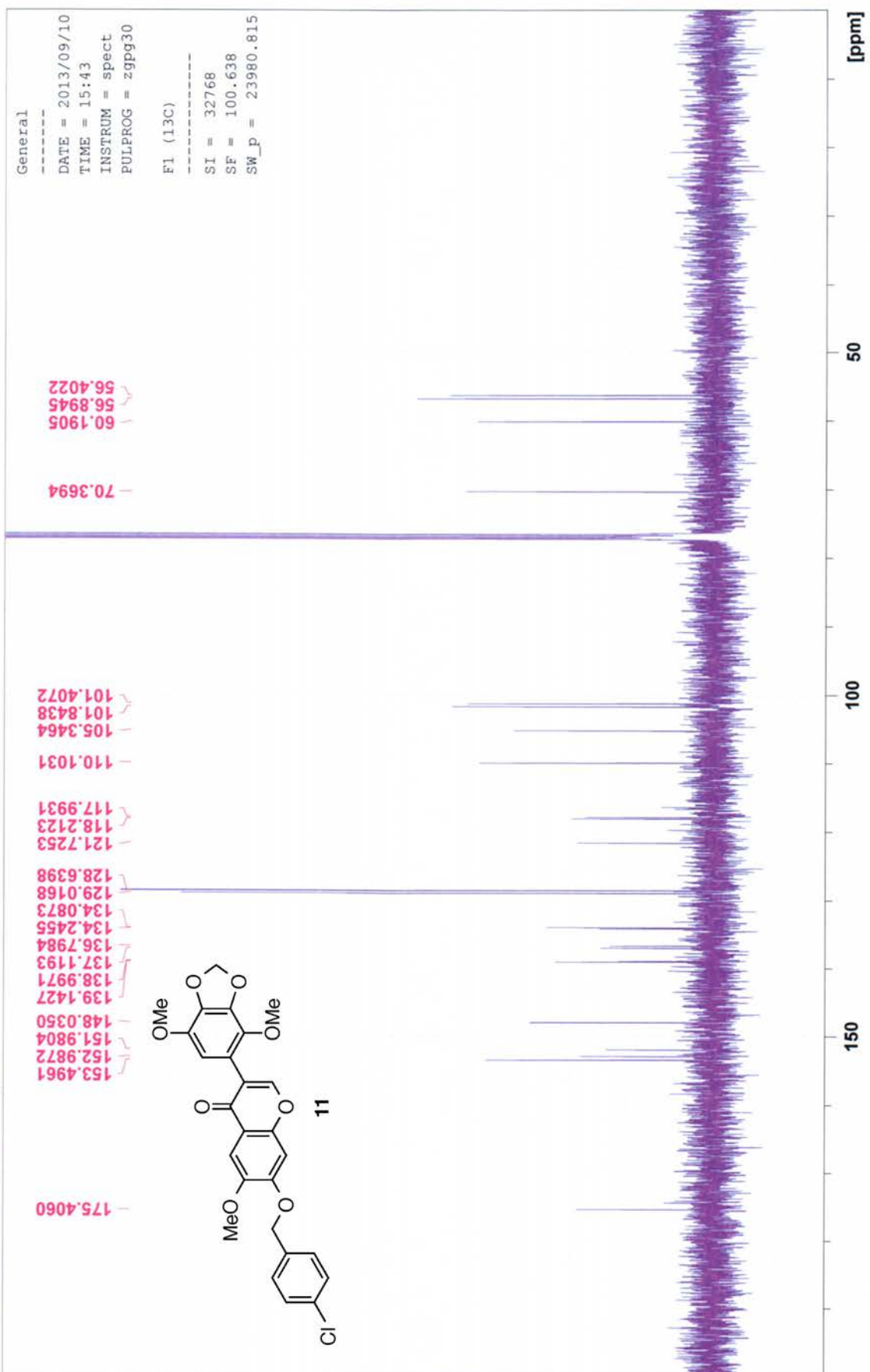
S1

ss-II-59 1 1 d: kigoshi

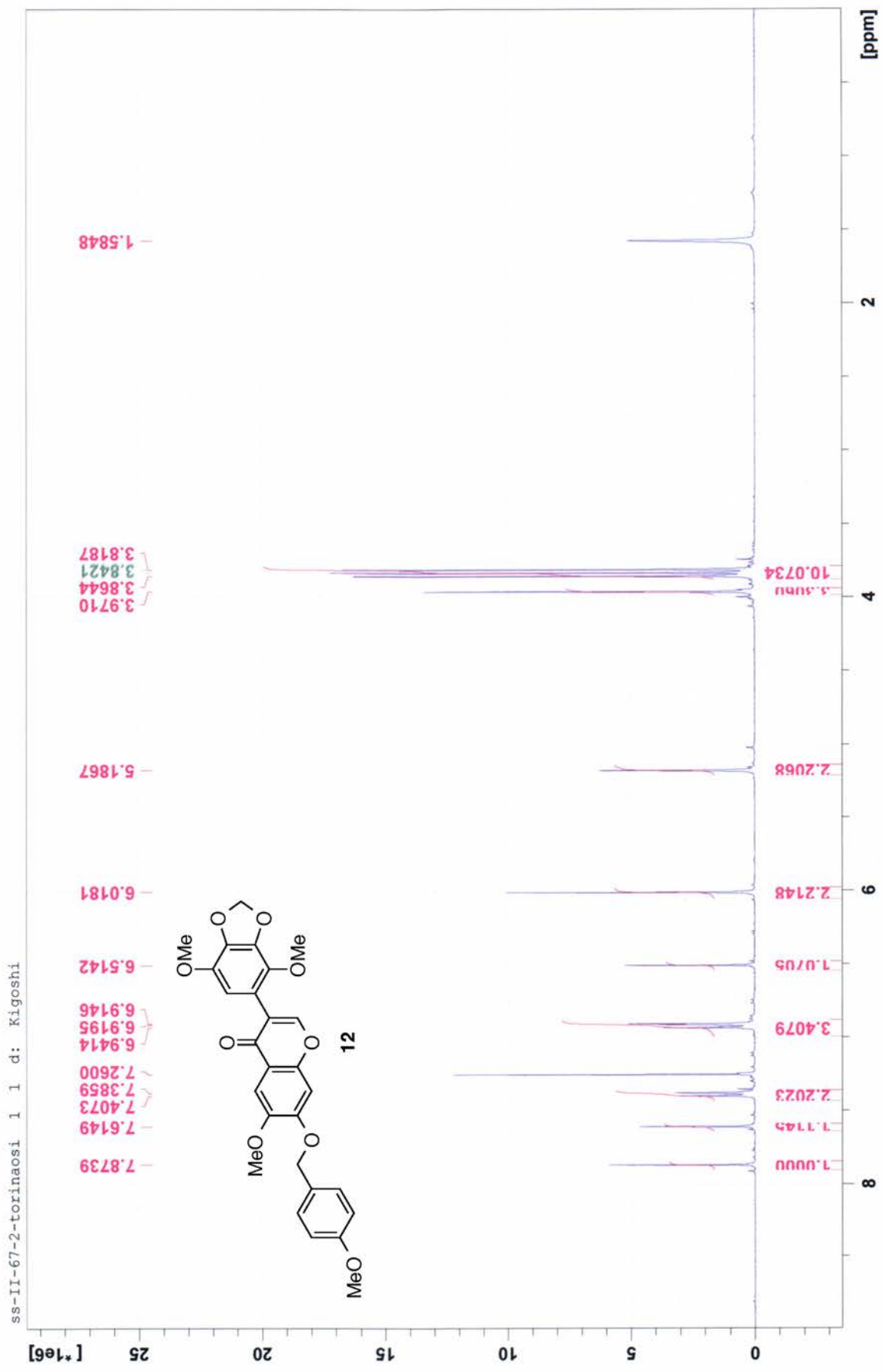


$^1\text{H}$  NMR spectra of **11** (400 MHz,  $\text{CDCl}_3$ )

ss-II-59-carbon 1 1 d: kigoshi

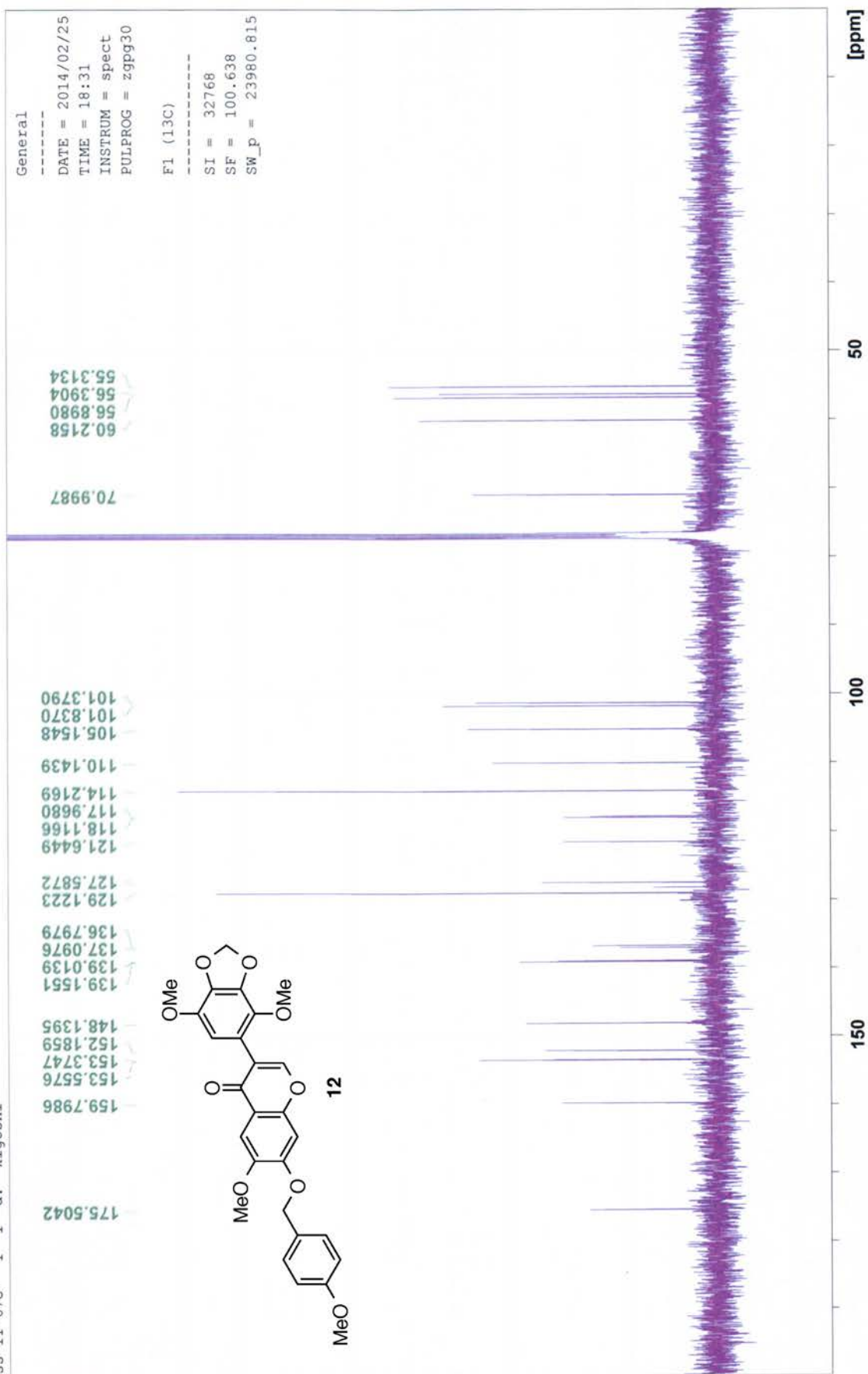


$^{13}\text{C}$  NMR spectra of **11** (100 MHz,  $\text{CDCl}_3$ )



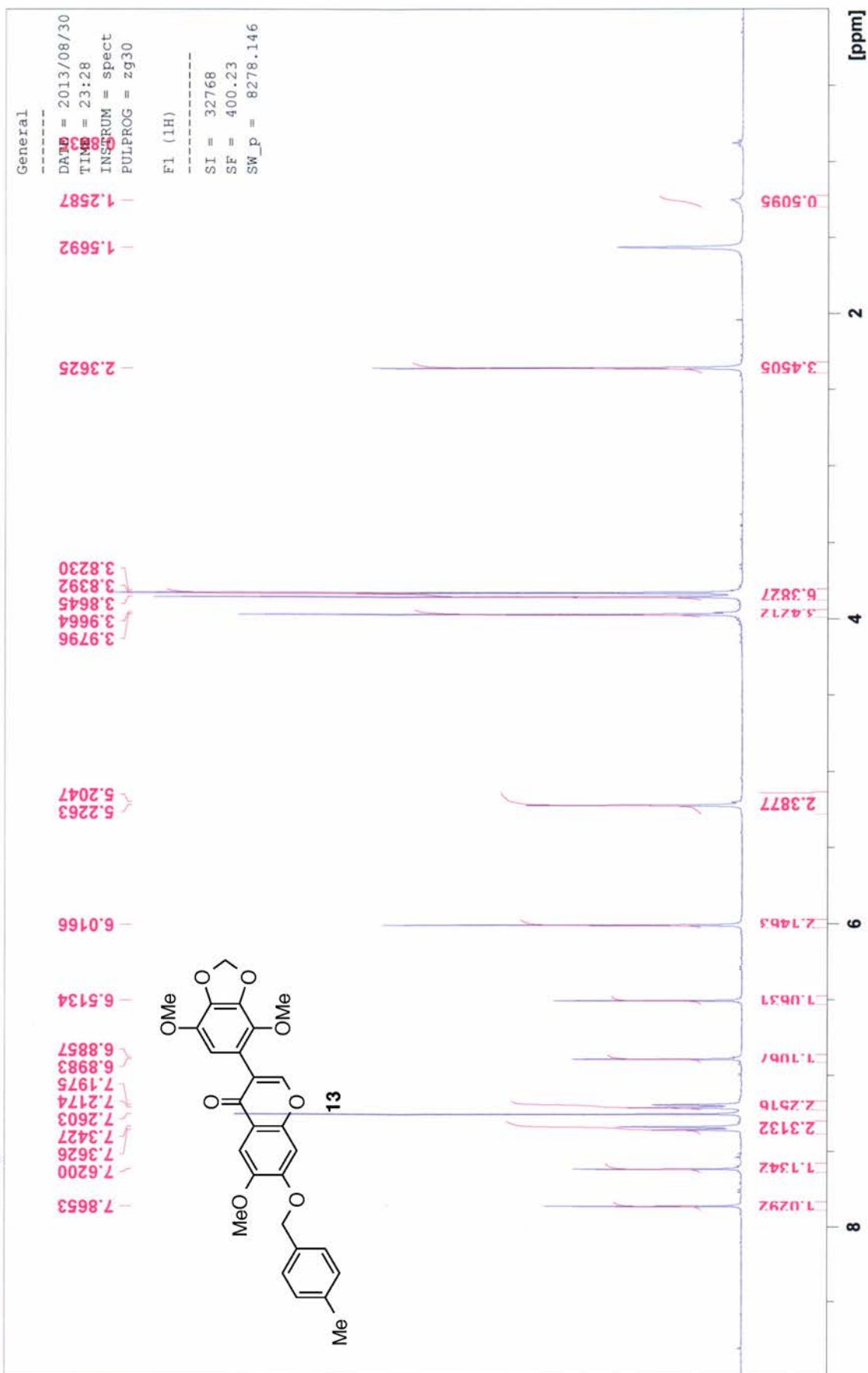
<sup>1</sup>H NMR spectra of **12** (400 MHz, CDCl<sub>3</sub>)

ss-II-67C' 1 1 d: kigoshi



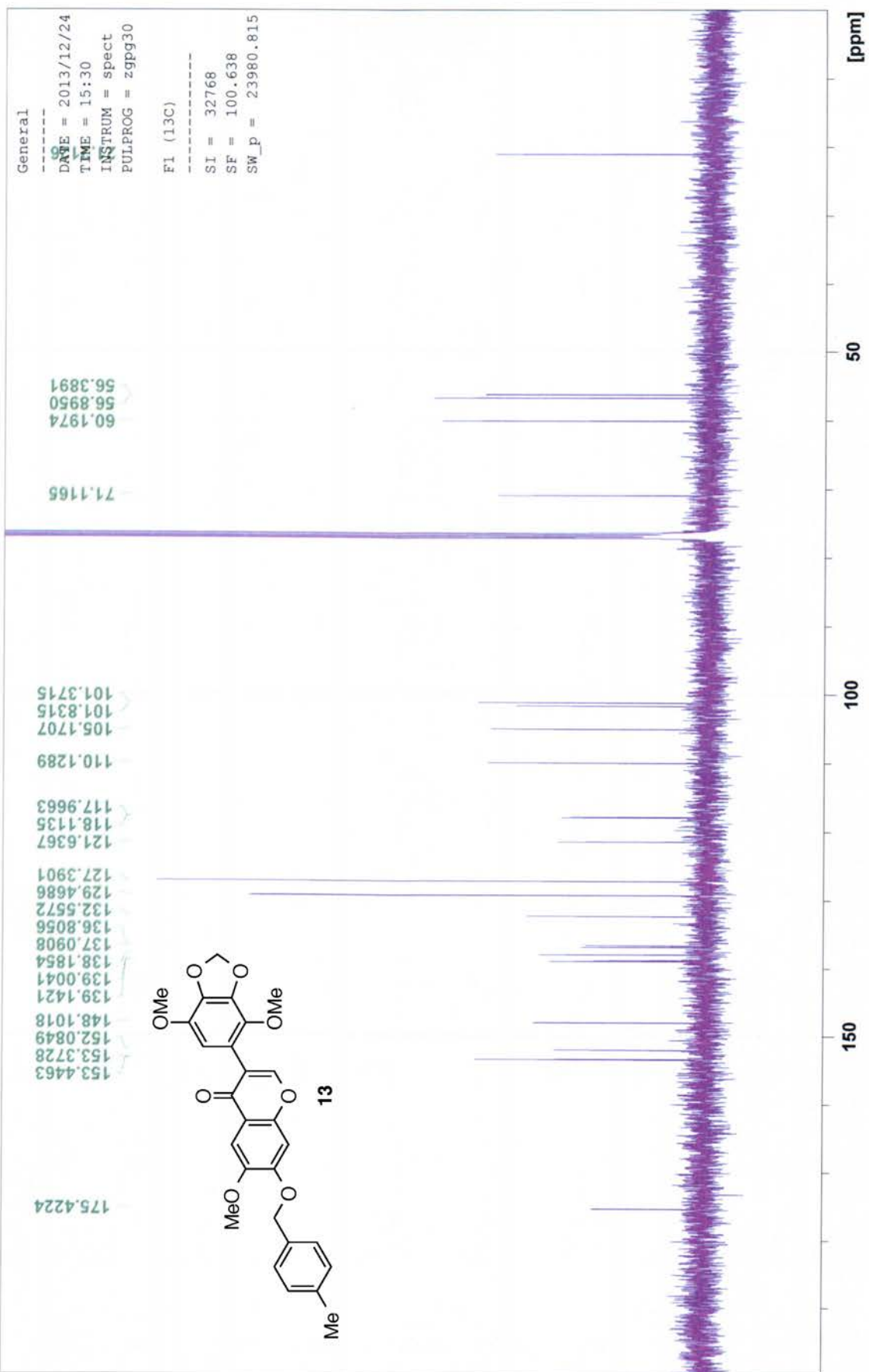
$^{13}\text{C}$  NMR spectra of **12** (100 MHz,  $\text{CDCl}_3$ )

ss-II-60 1 1 d: kigoshi



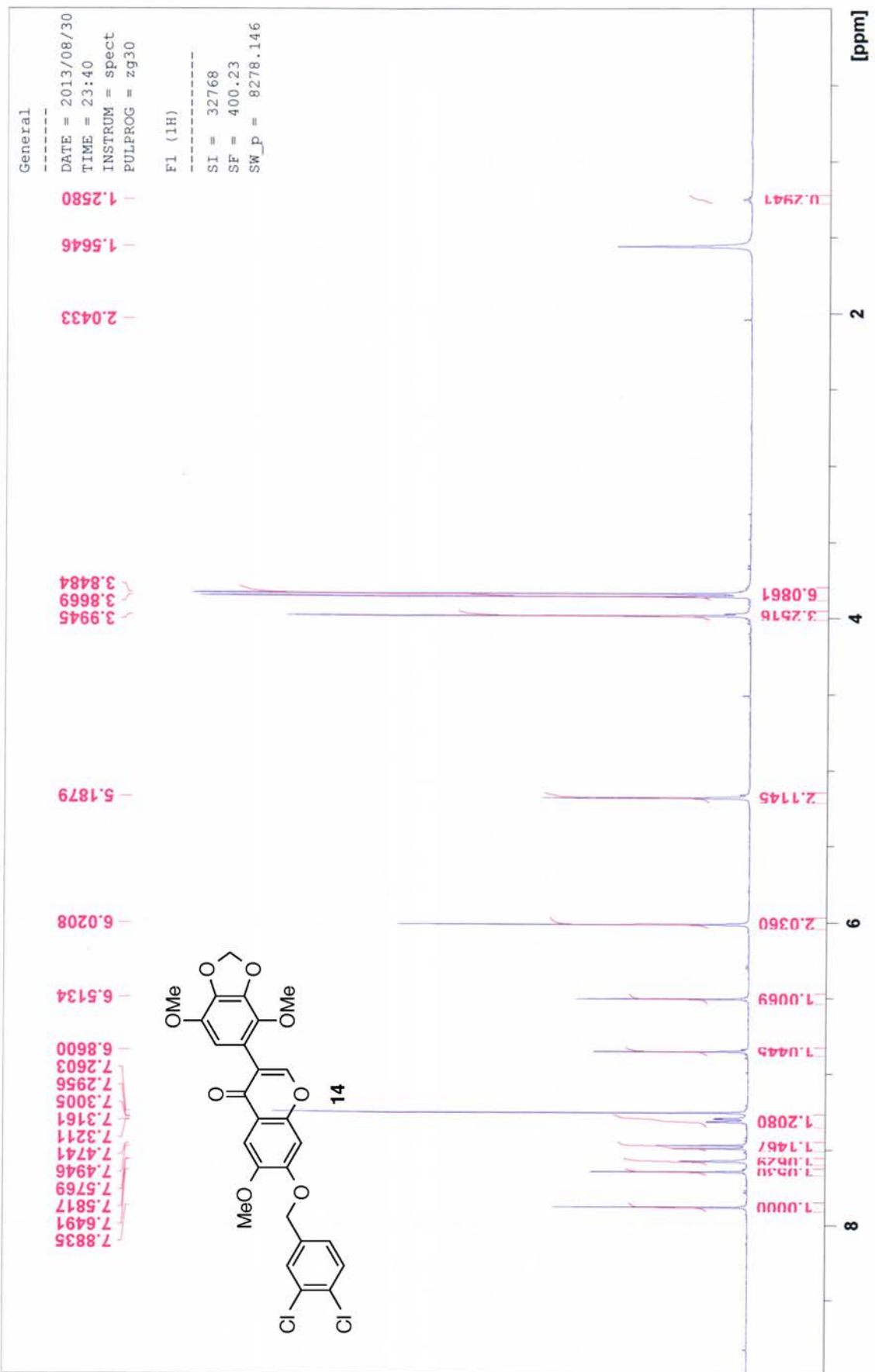
$^1\text{H}$  NMR spectra of **13** (400 MHz,  $\text{CDCl}_3$ )

ss-II-60-C 1 1 d: kigoshi



$^{13}\text{C}$  NMR spectra of **13** (100 MHz,  $\text{CDCl}_3$ )

ss-II-61 1 1 d: kigoshi

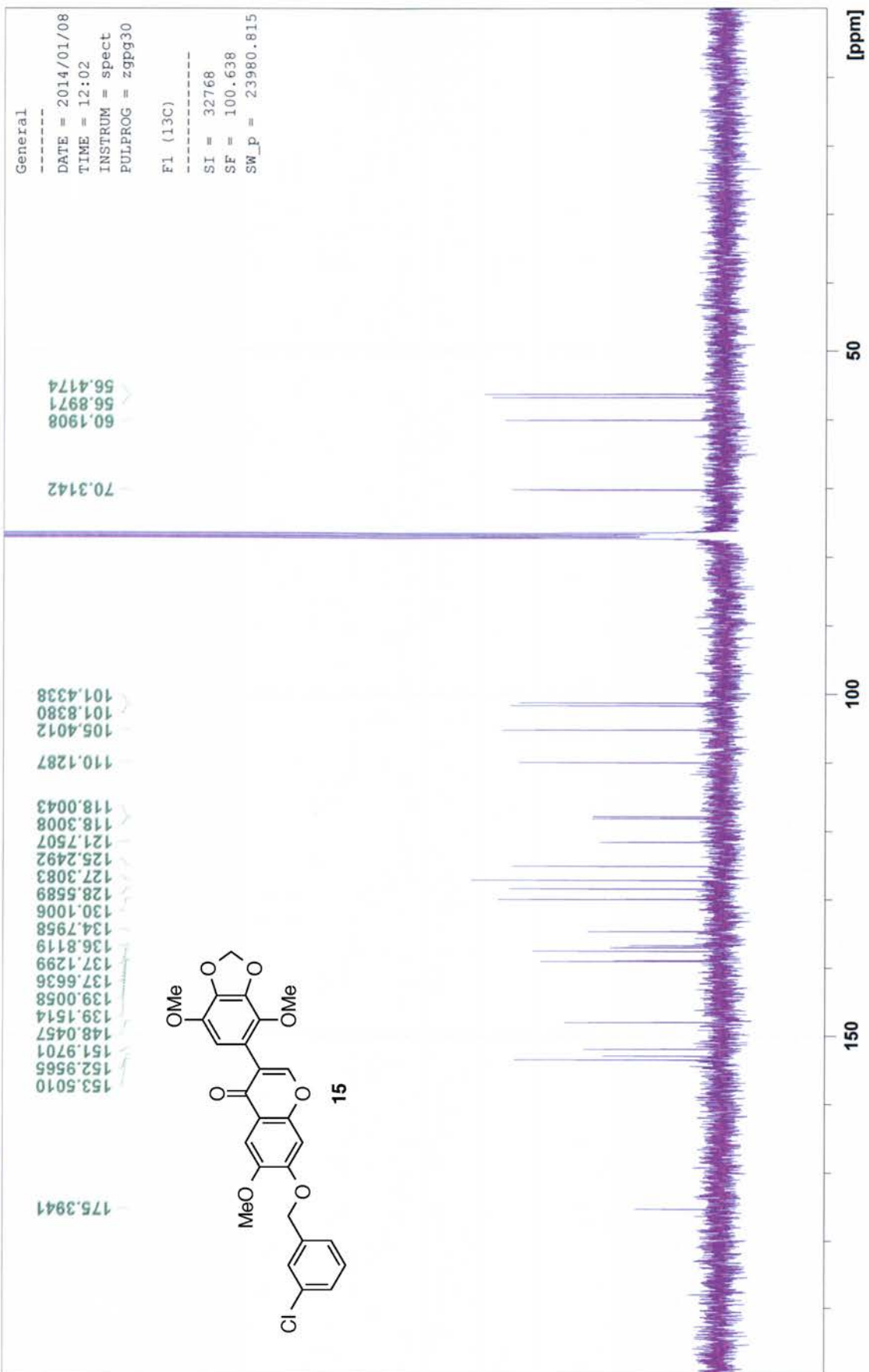


$^1\text{H}$  NMR spectra of **14** (400 MHz,  $\text{CDCl}_3$ )



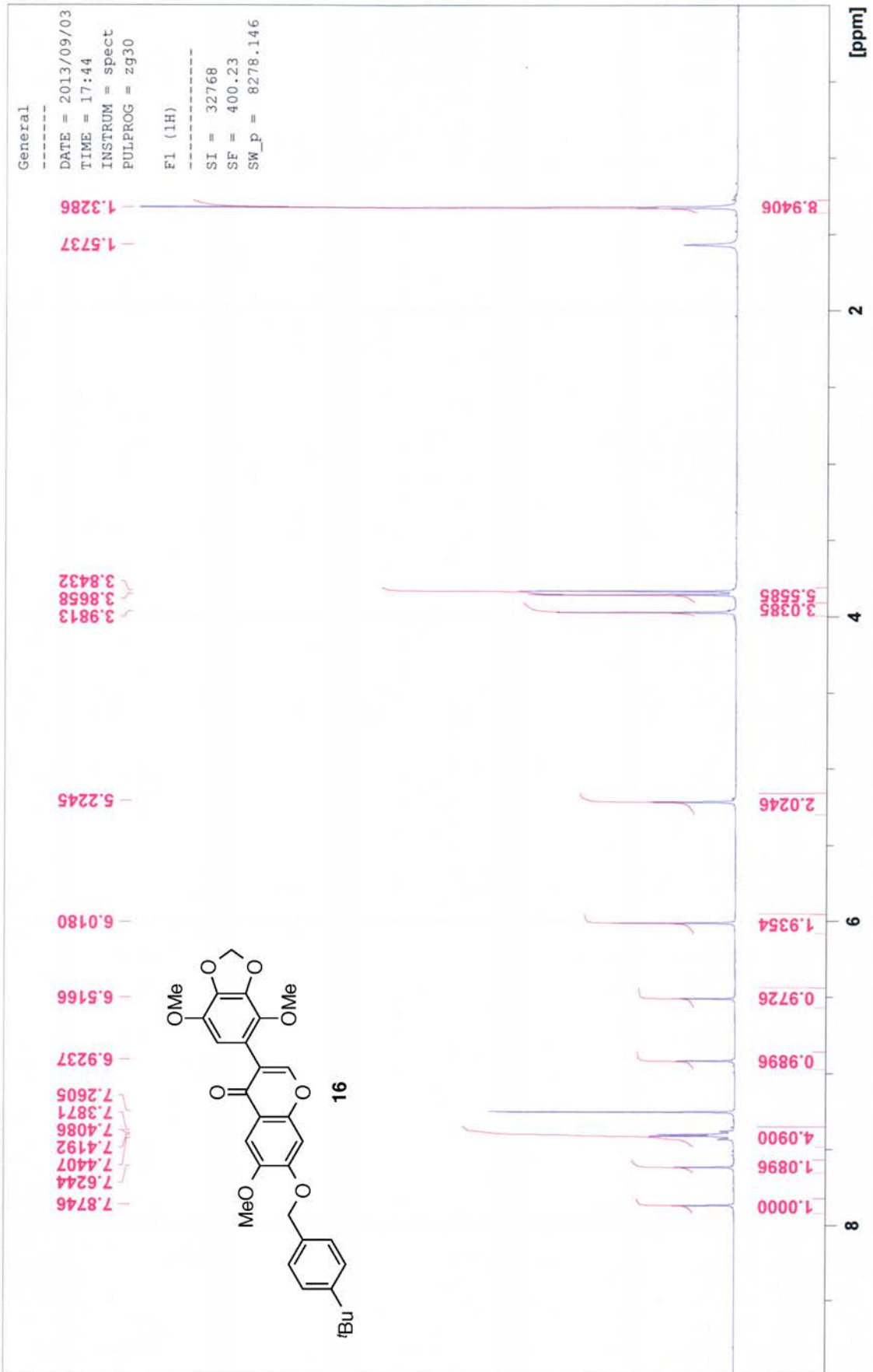


ss-II-62C 1 1 d: kigoshi



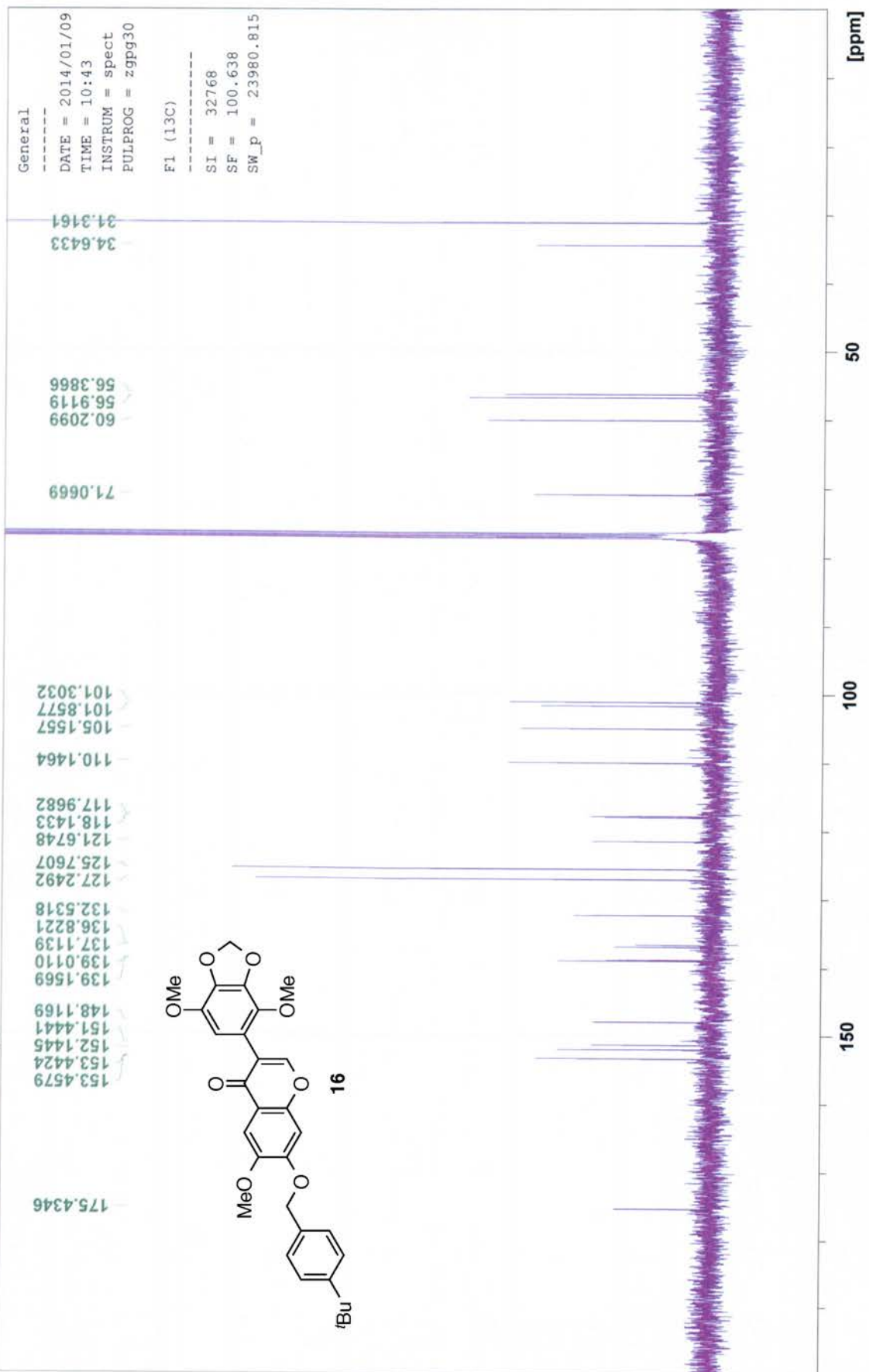
$^{13}\text{C}$  NMR spectra of **15** (100 MHz,  $\text{CDCl}_3$ )

ss-II-63 1 1 d: kigoshi



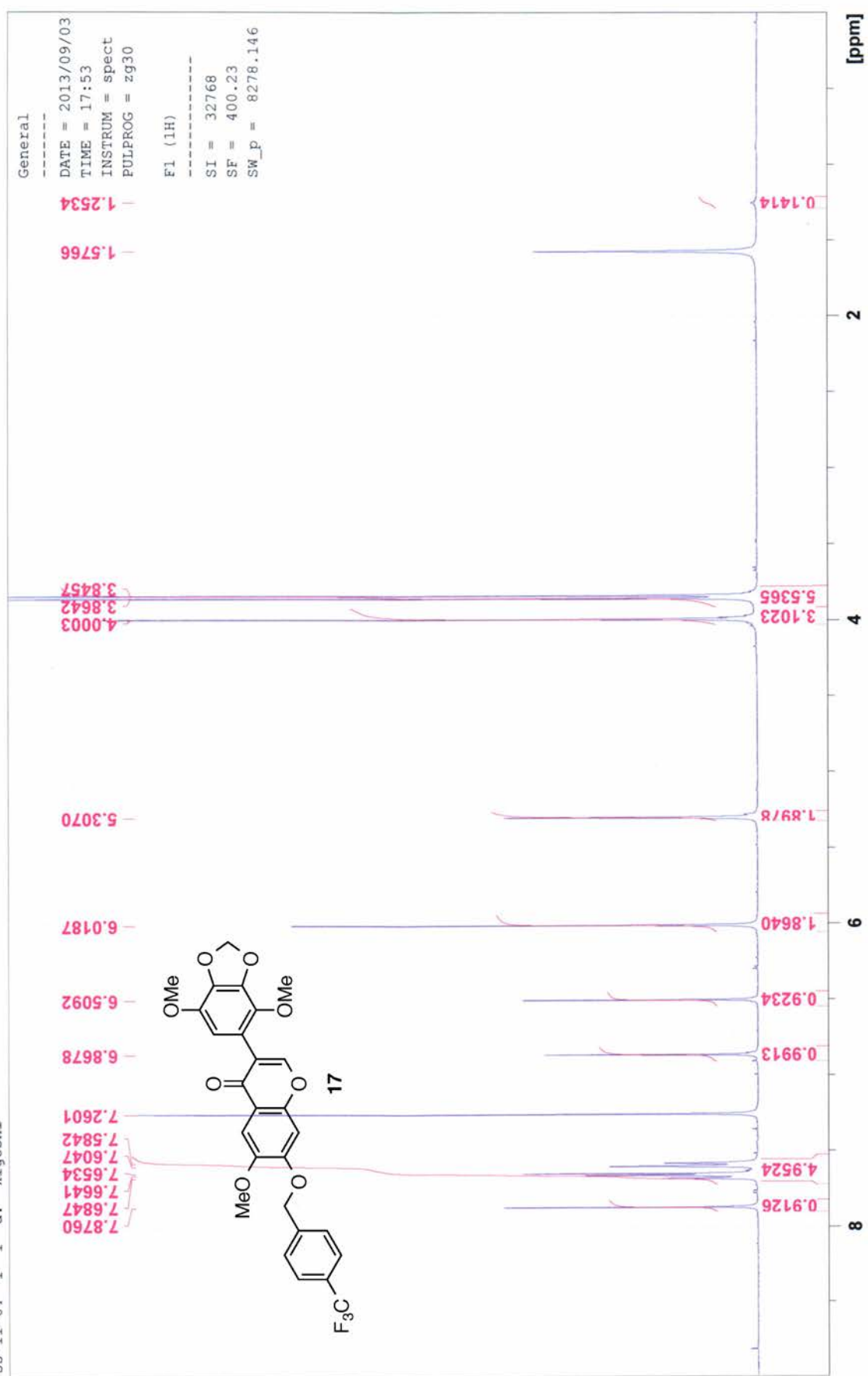
$^1\text{H}$  NMR spectra of **16** (400 MHz,  $\text{CDCl}_3$ )

ss-II-63C(torinaosi) 1 1 d: kigoshi



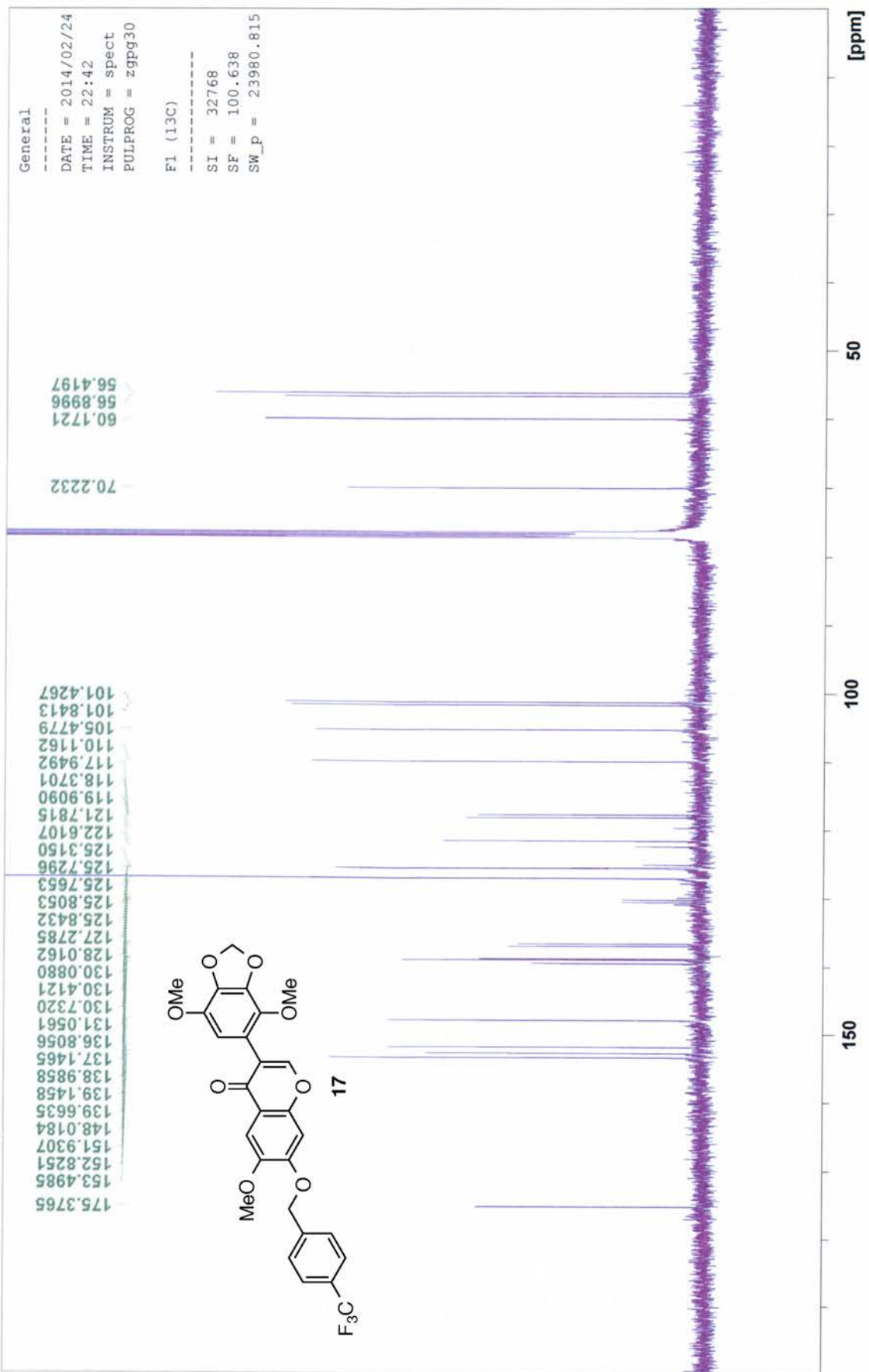
<sup>13</sup>C NMR spectra of **16** (100 MHz, CDCl<sub>3</sub>)

ss-II-64 1 1 d: kigoshi

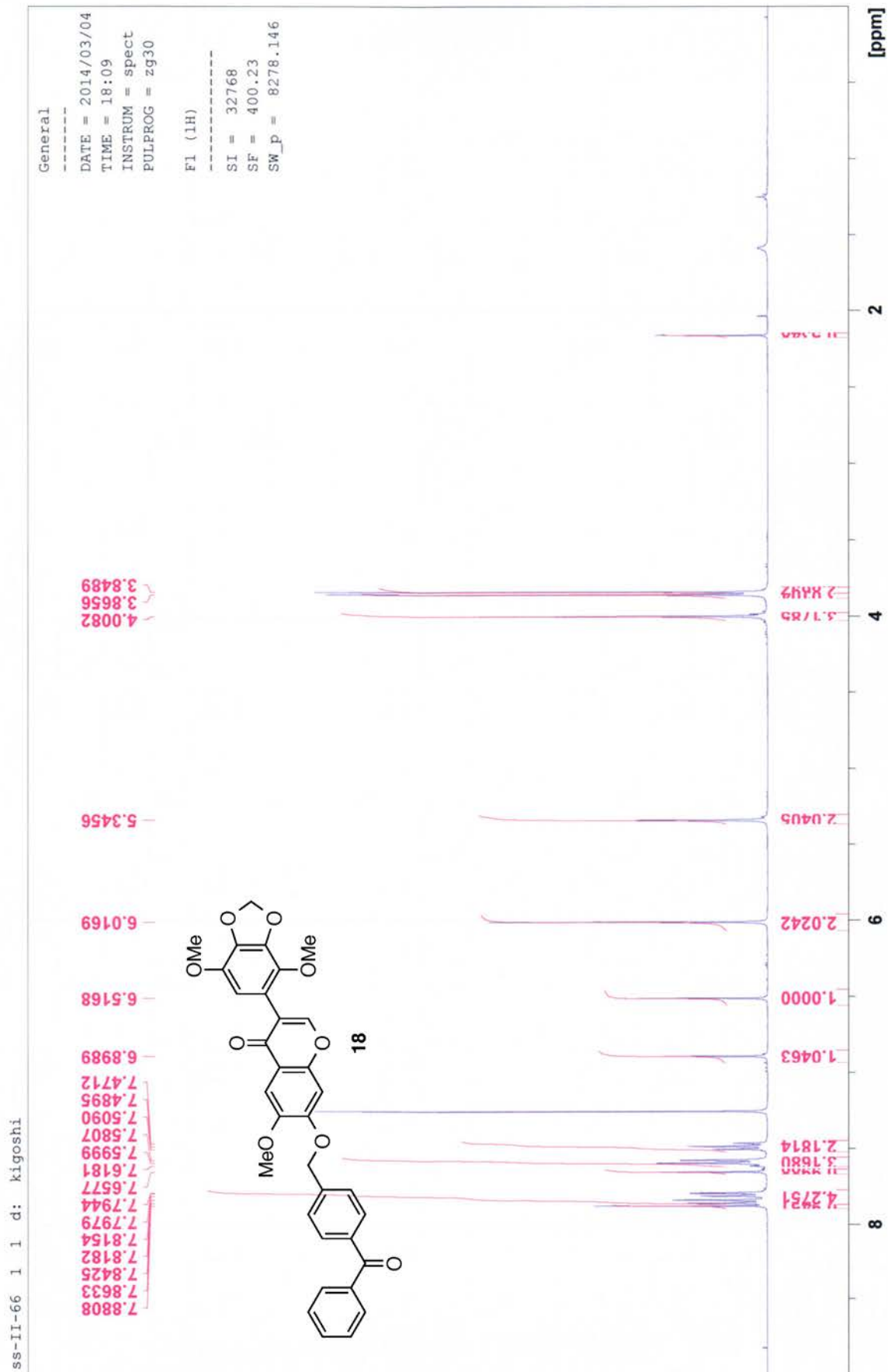


$^1\text{H}$  NMR spectra of **17** (400 MHz,  $\text{CDCl}_3$ )

SS-II-64C' 1 1 d: kigoshi

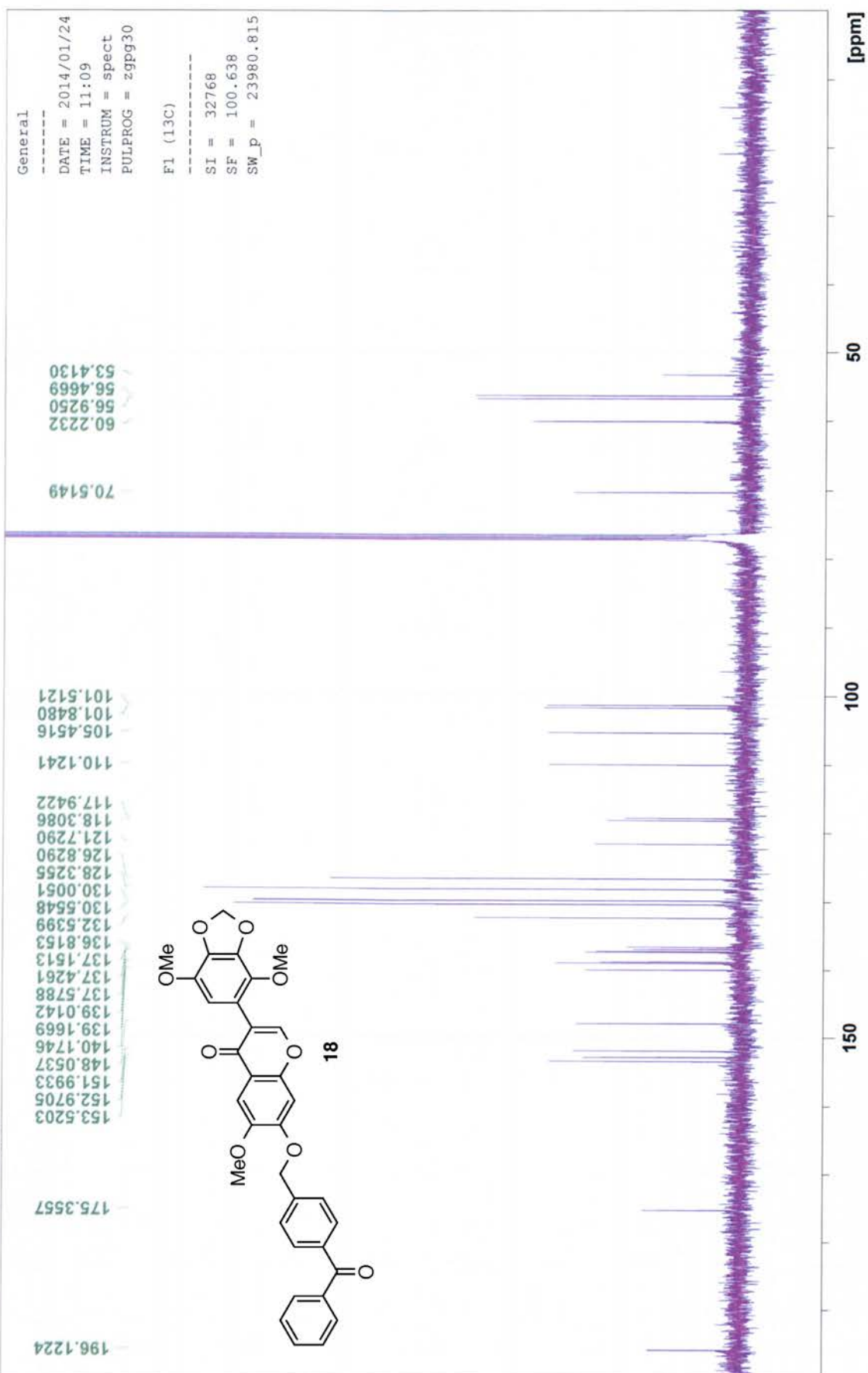


$^{13}\text{C}$  NMR spectra of **17** (100 MHz,  $\text{CDCl}_3$ )



$^1\text{H}$  NMR spectra of **18** (400 MHz,  $\text{CDCl}_3$ )

ss-II-66C 1 1 d: kigoshi



$^{13}\text{C}$  NMR spectra of **18** (100 MHz,  $\text{CDCl}_3$ )