Supporting Information

Identification of potent chromone embedded [1,2,3]-triazoles as novel antitubercular agents

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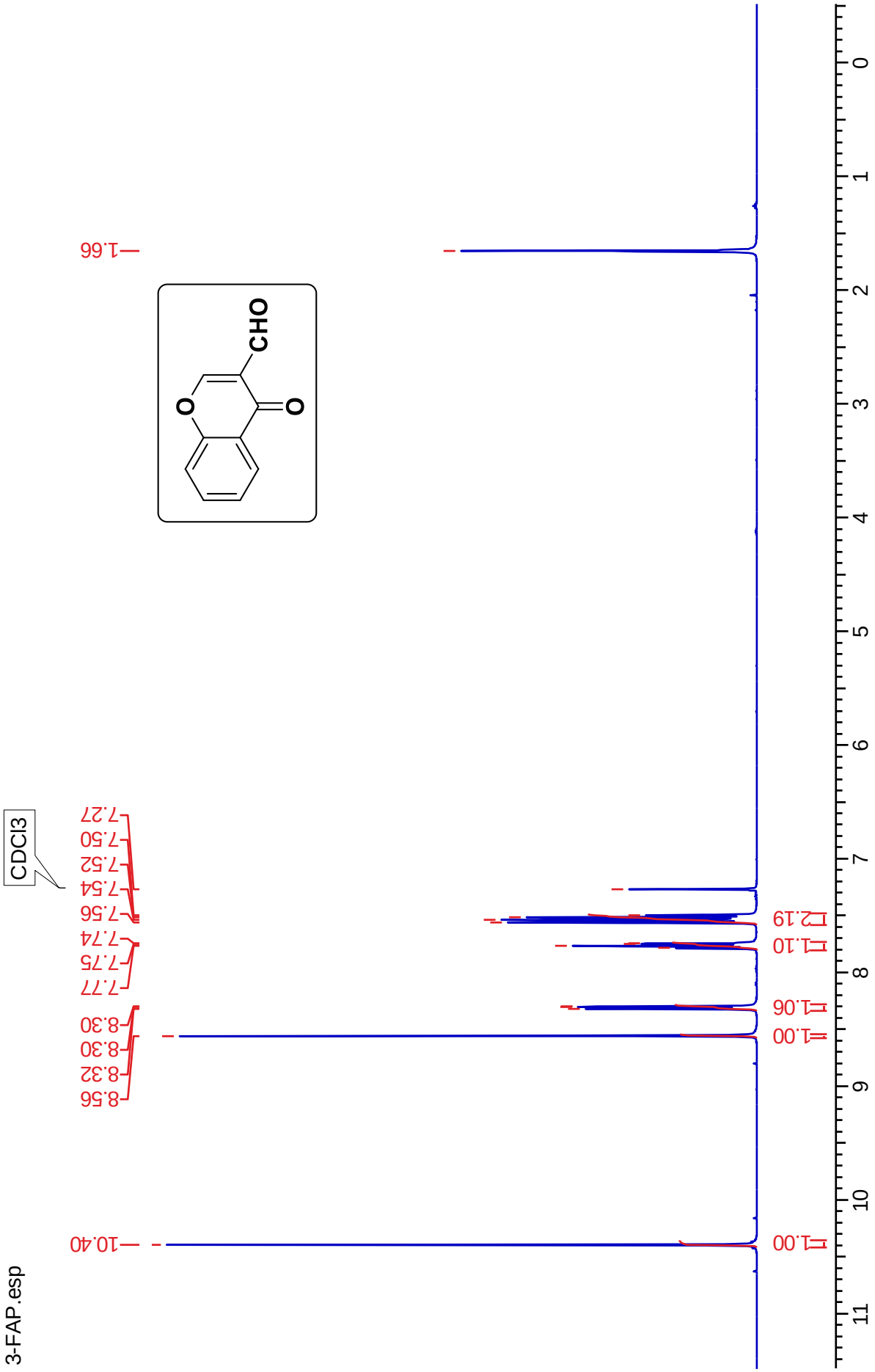
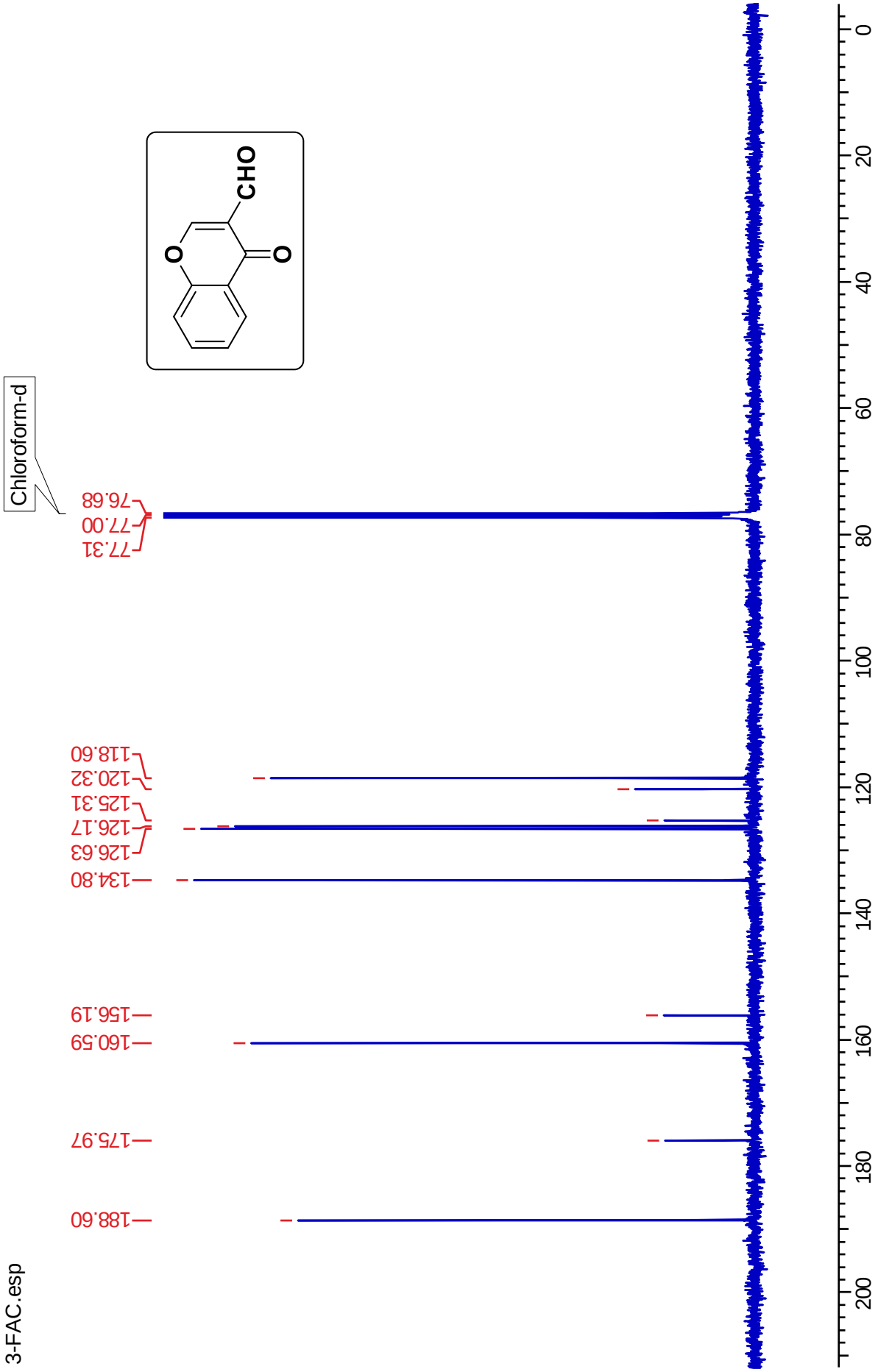
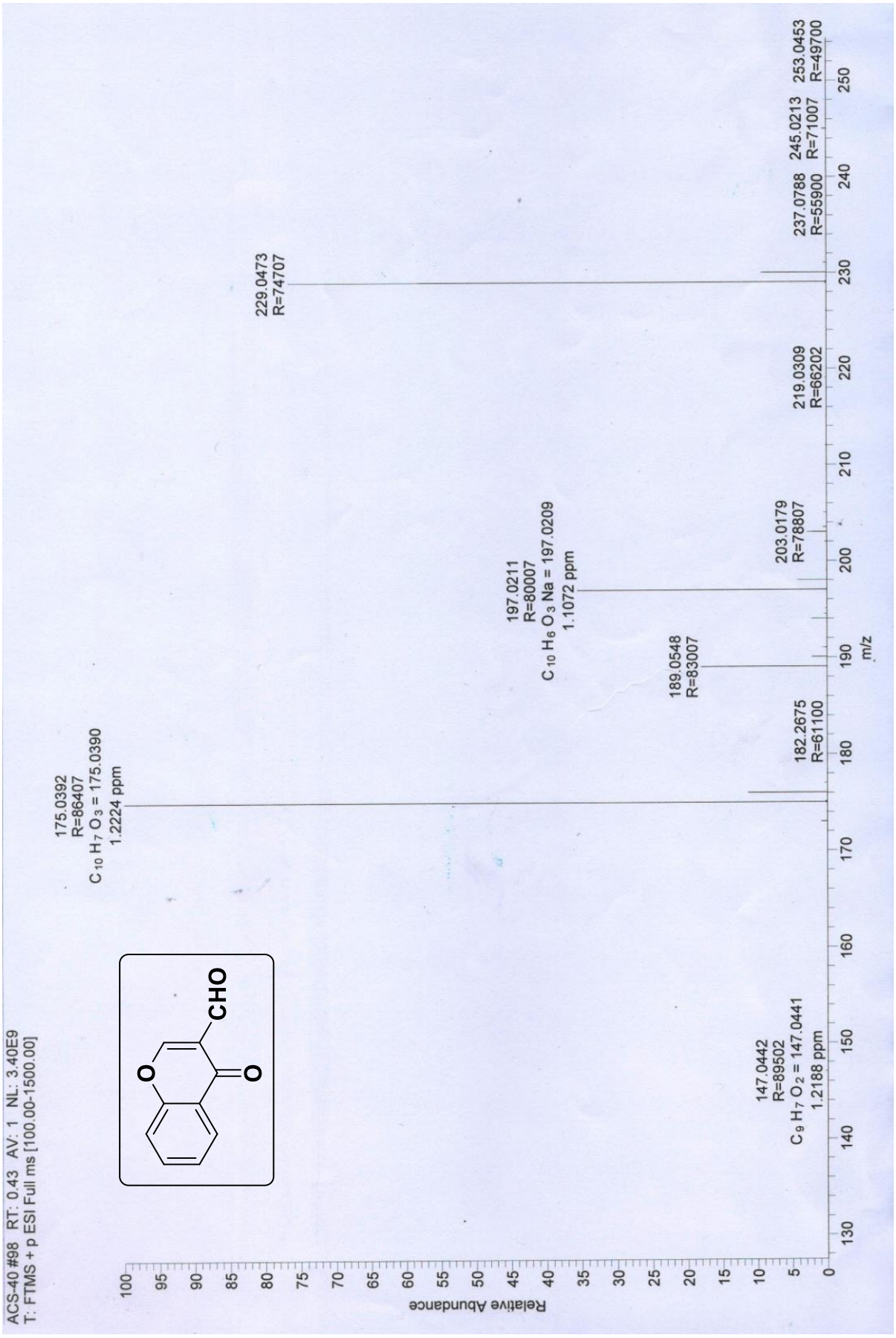
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***2***:



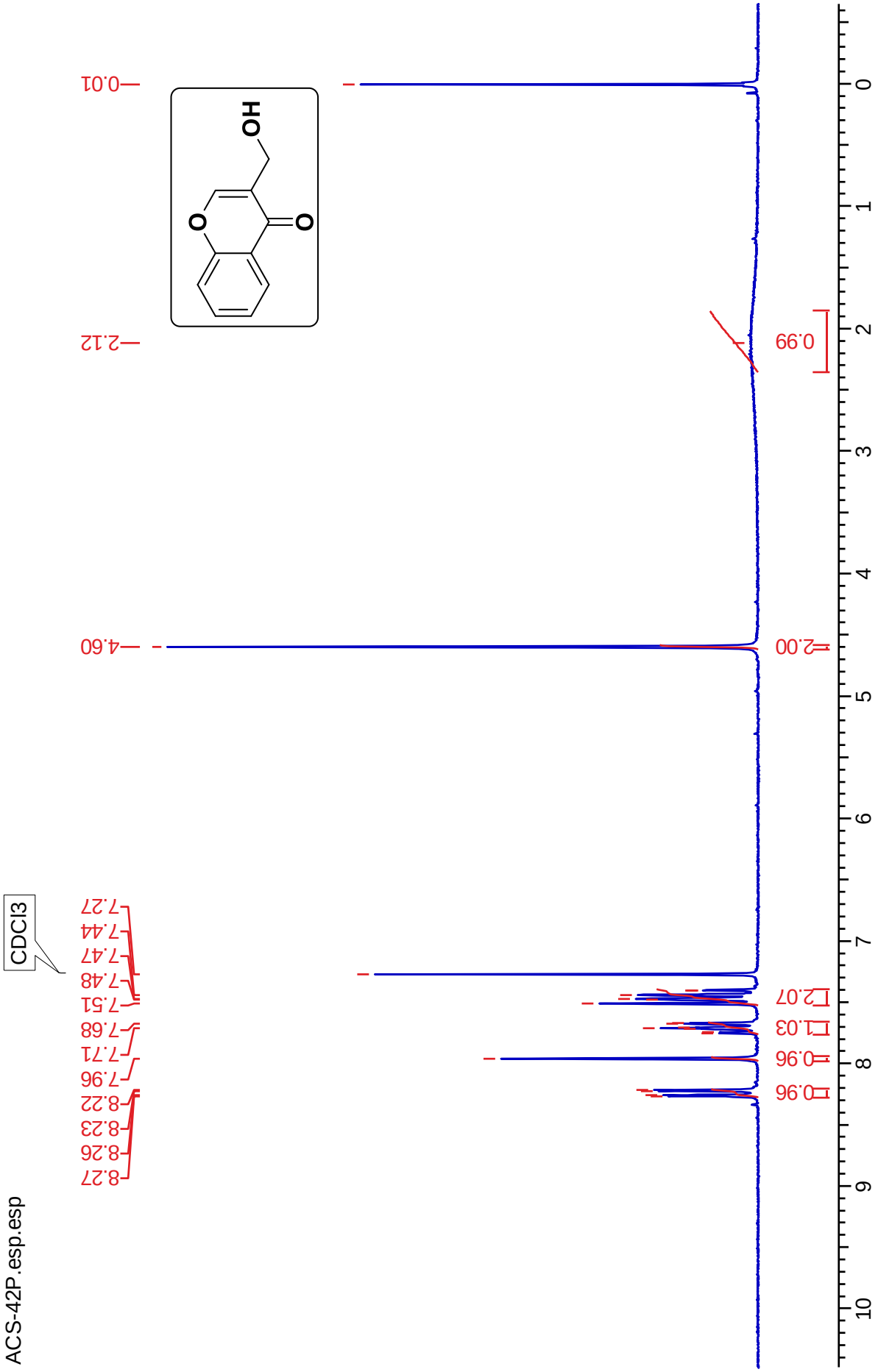
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***2***:



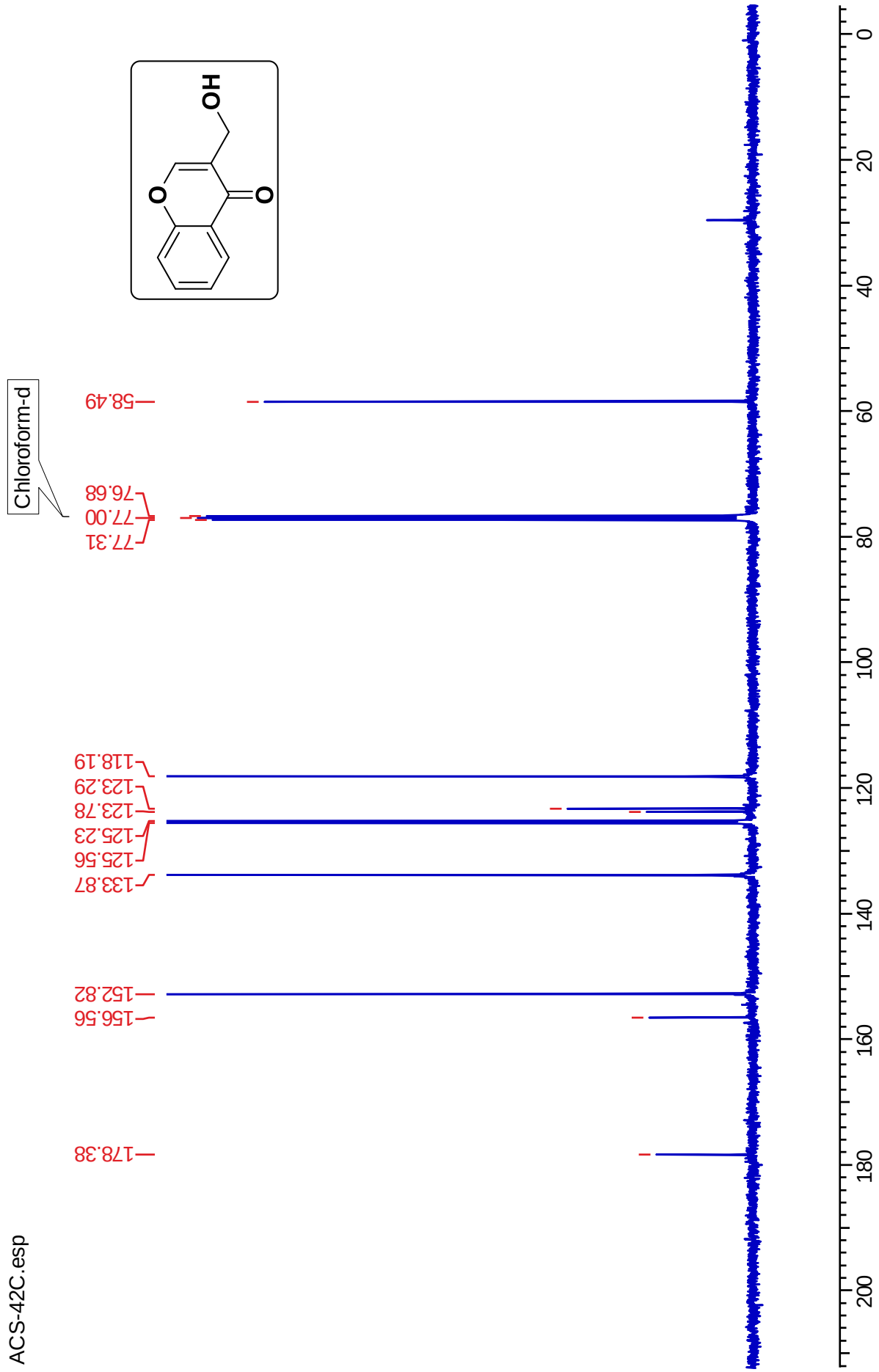
HRMS of compound ***2***:



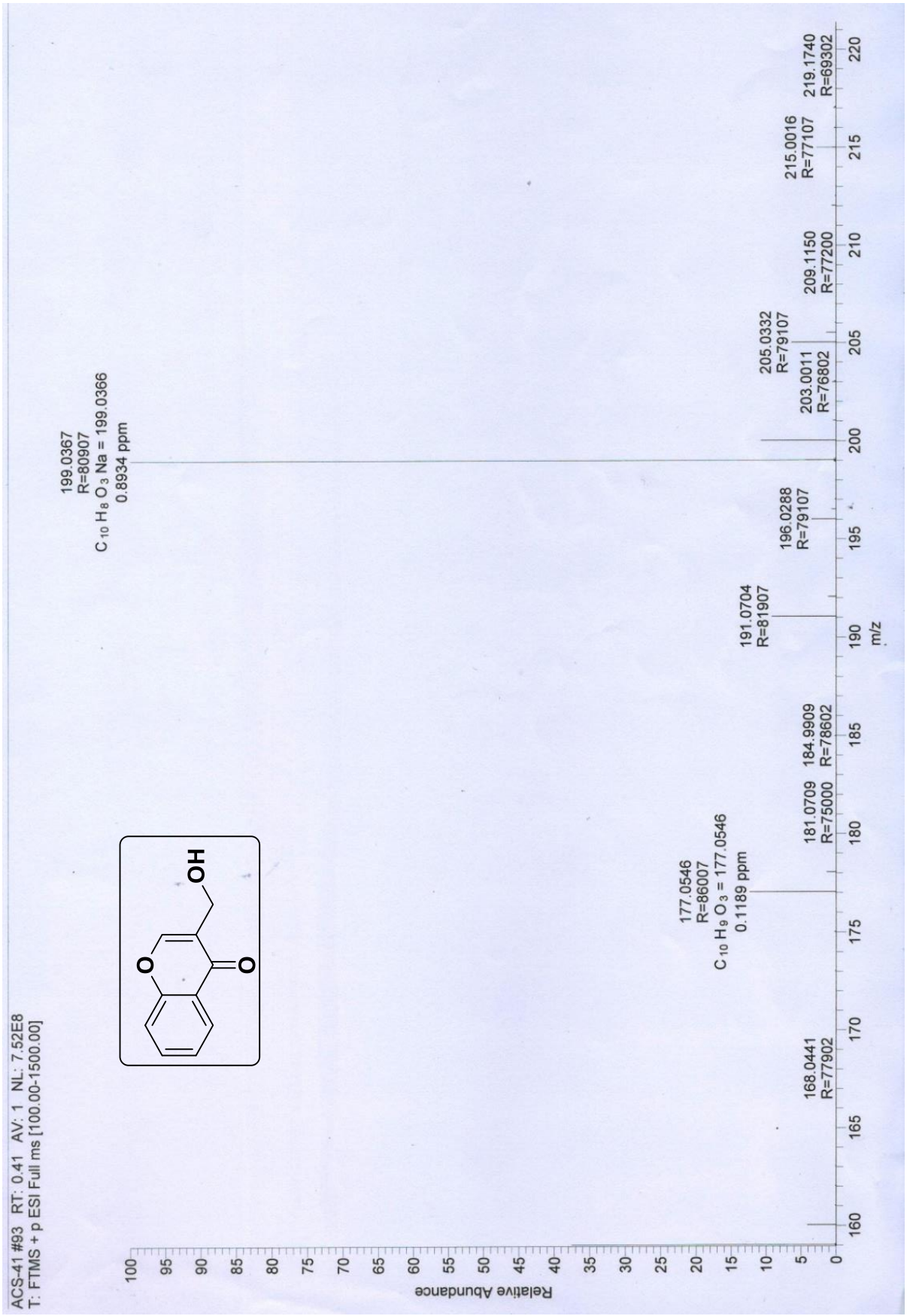
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3**:



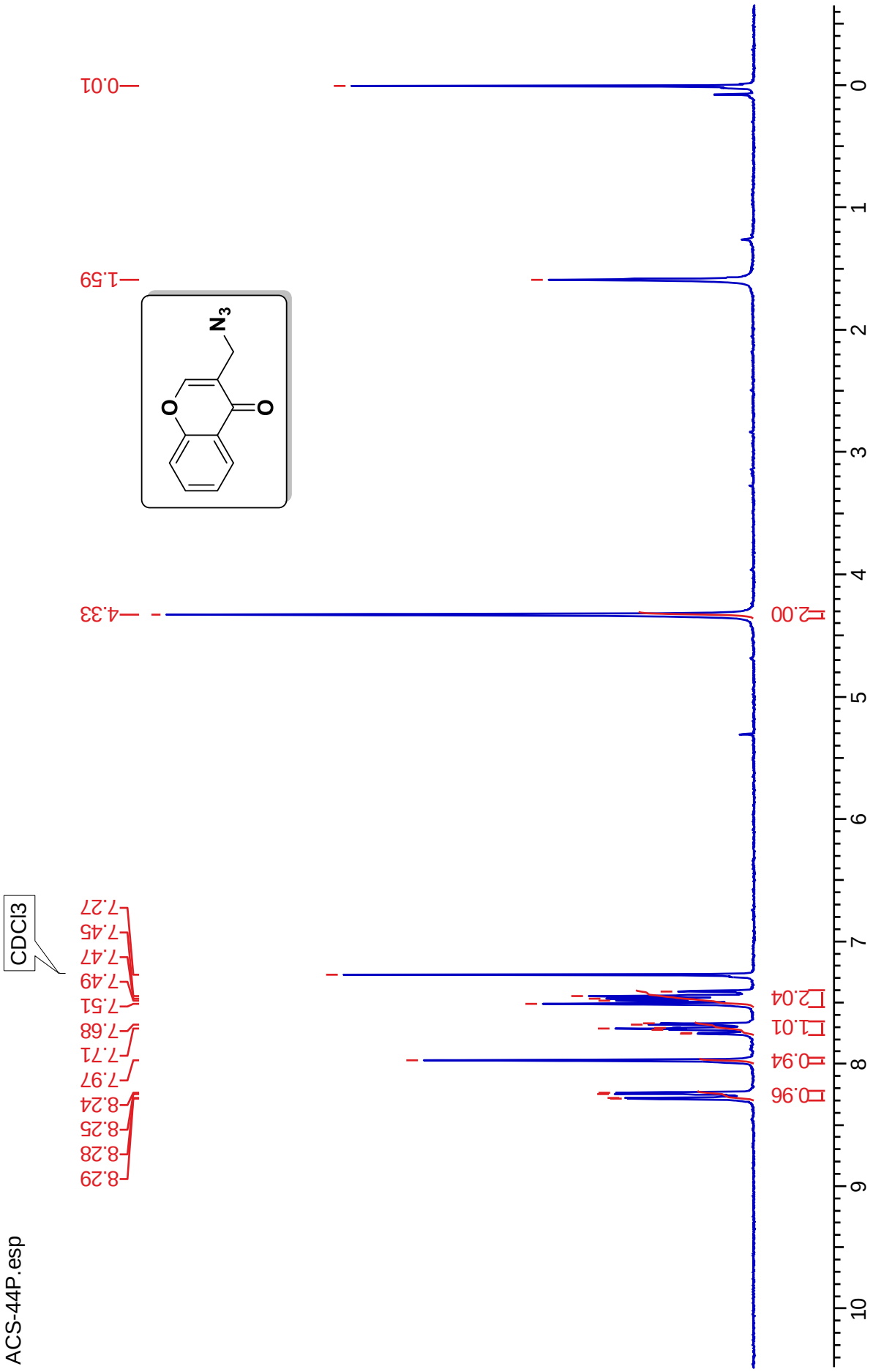
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***3***:



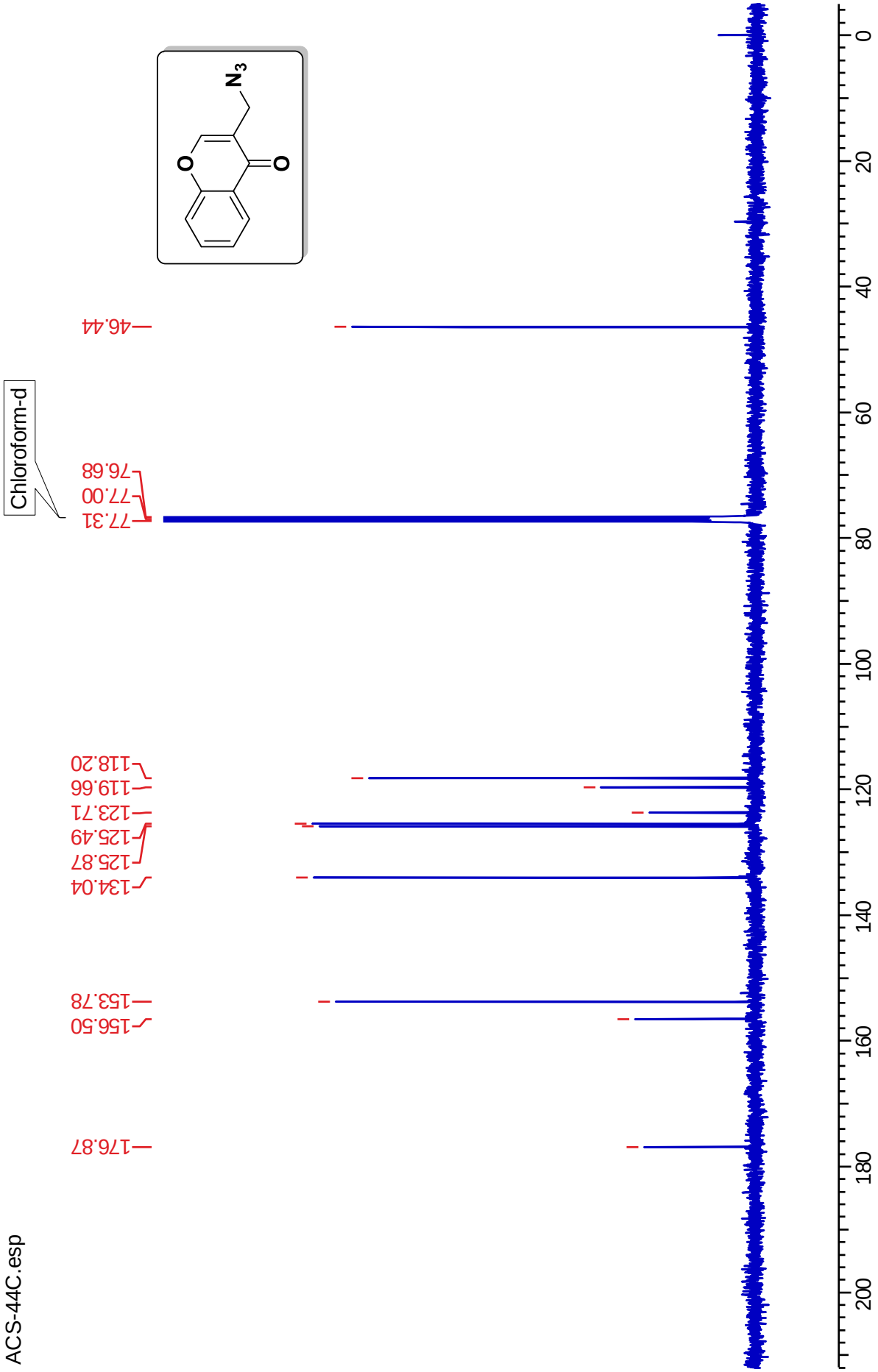
HRMS of compound ***3***:



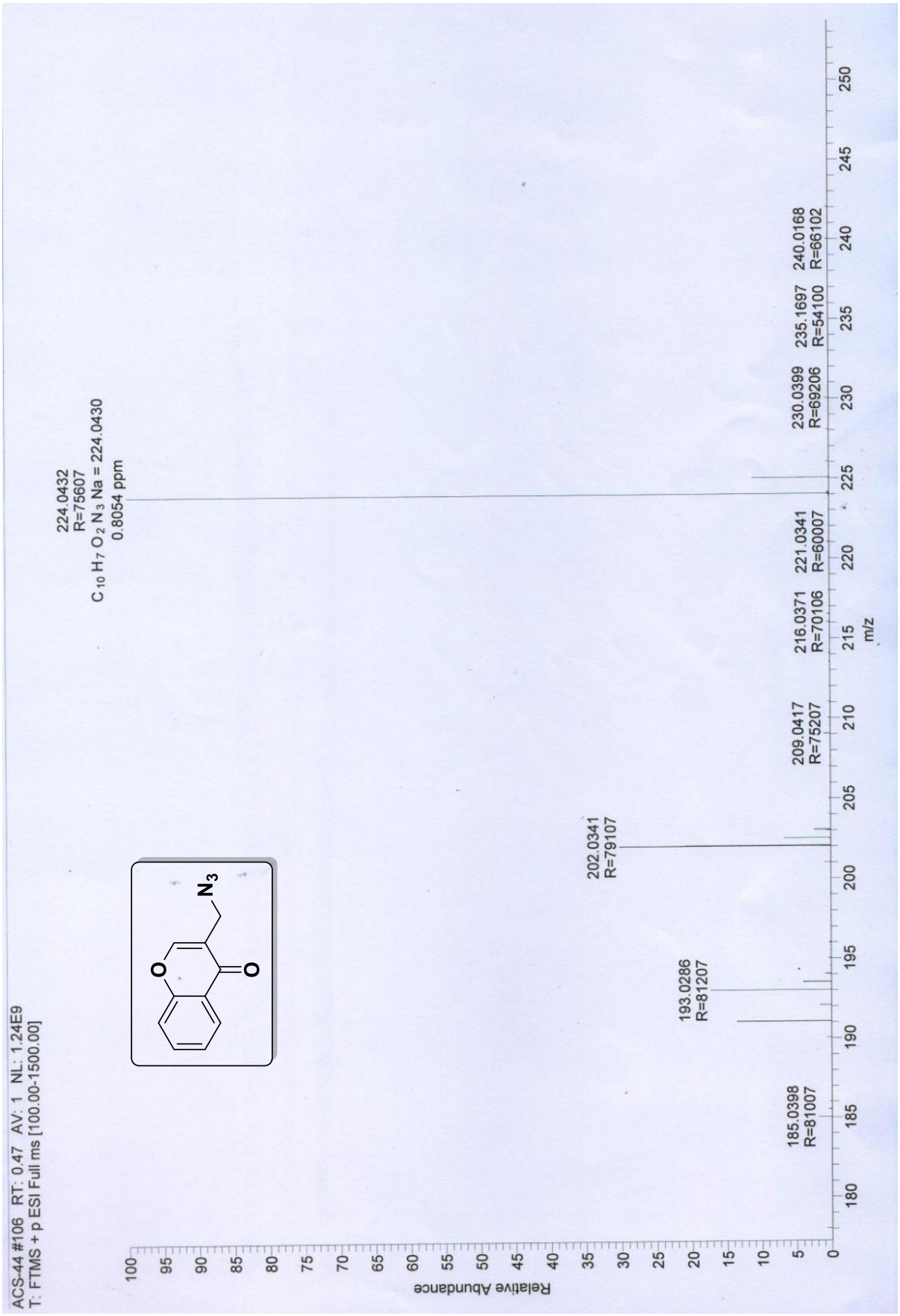
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***4***:



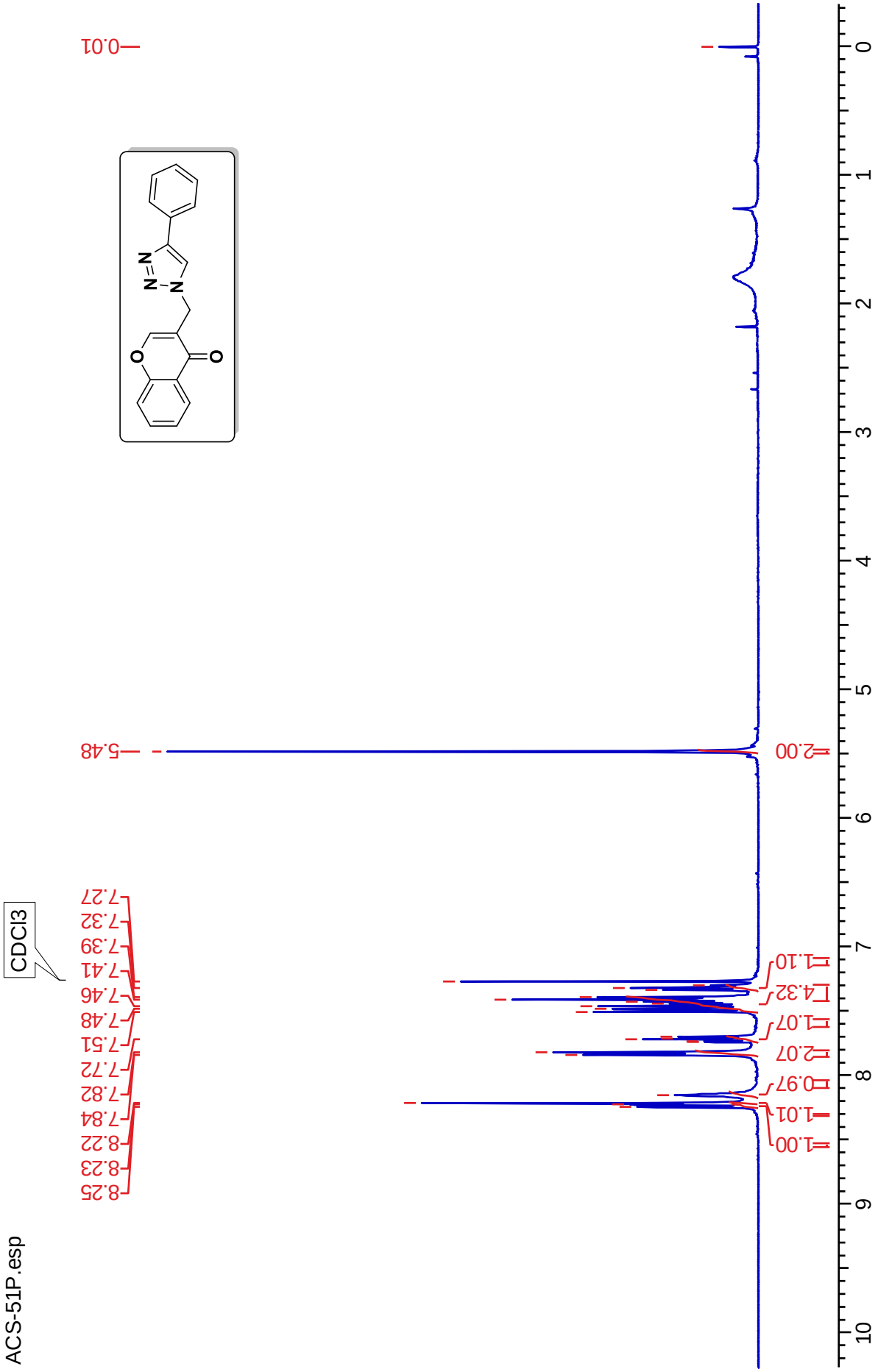
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***4***:



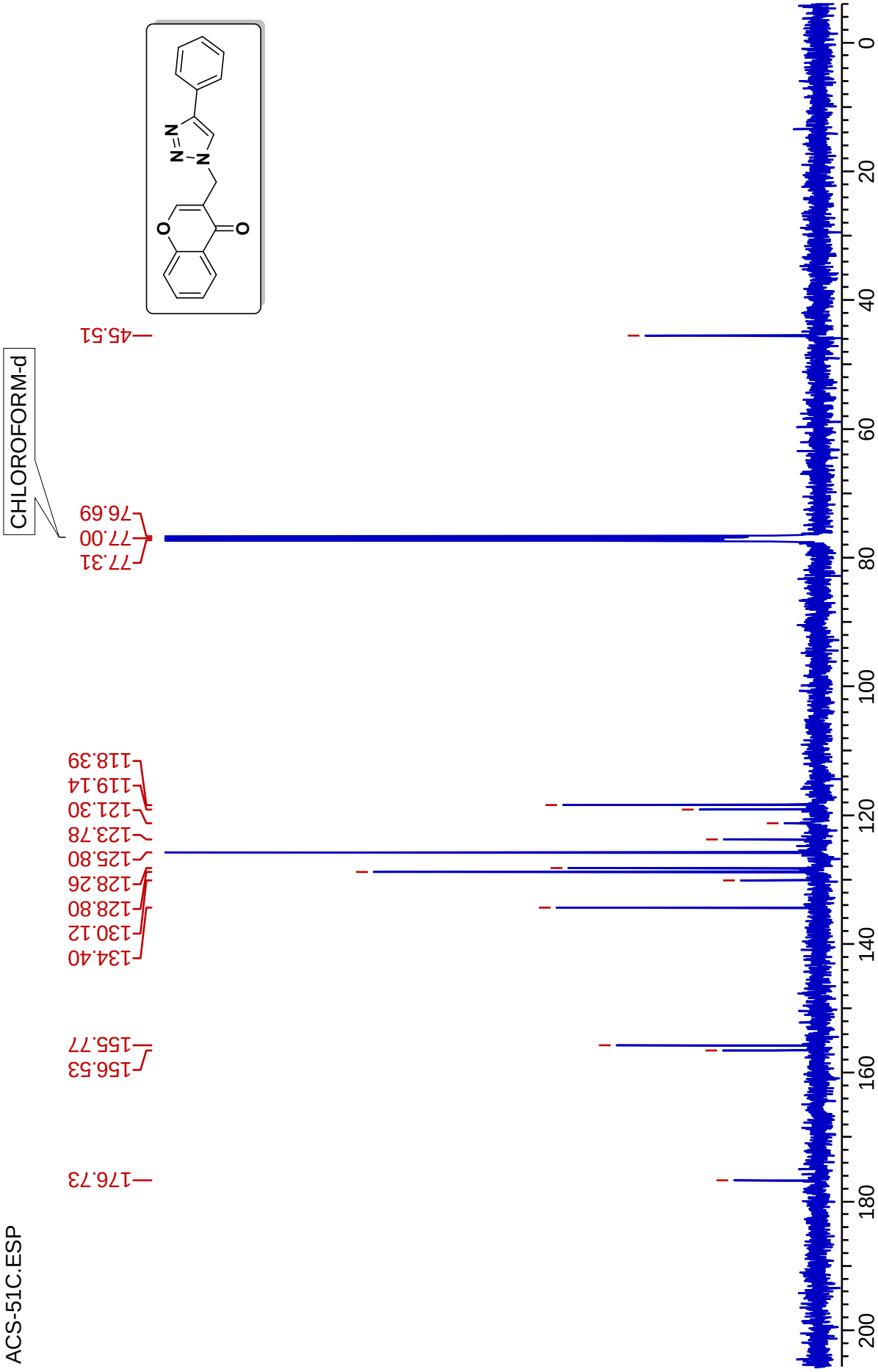
HRMS of compound ***4***:



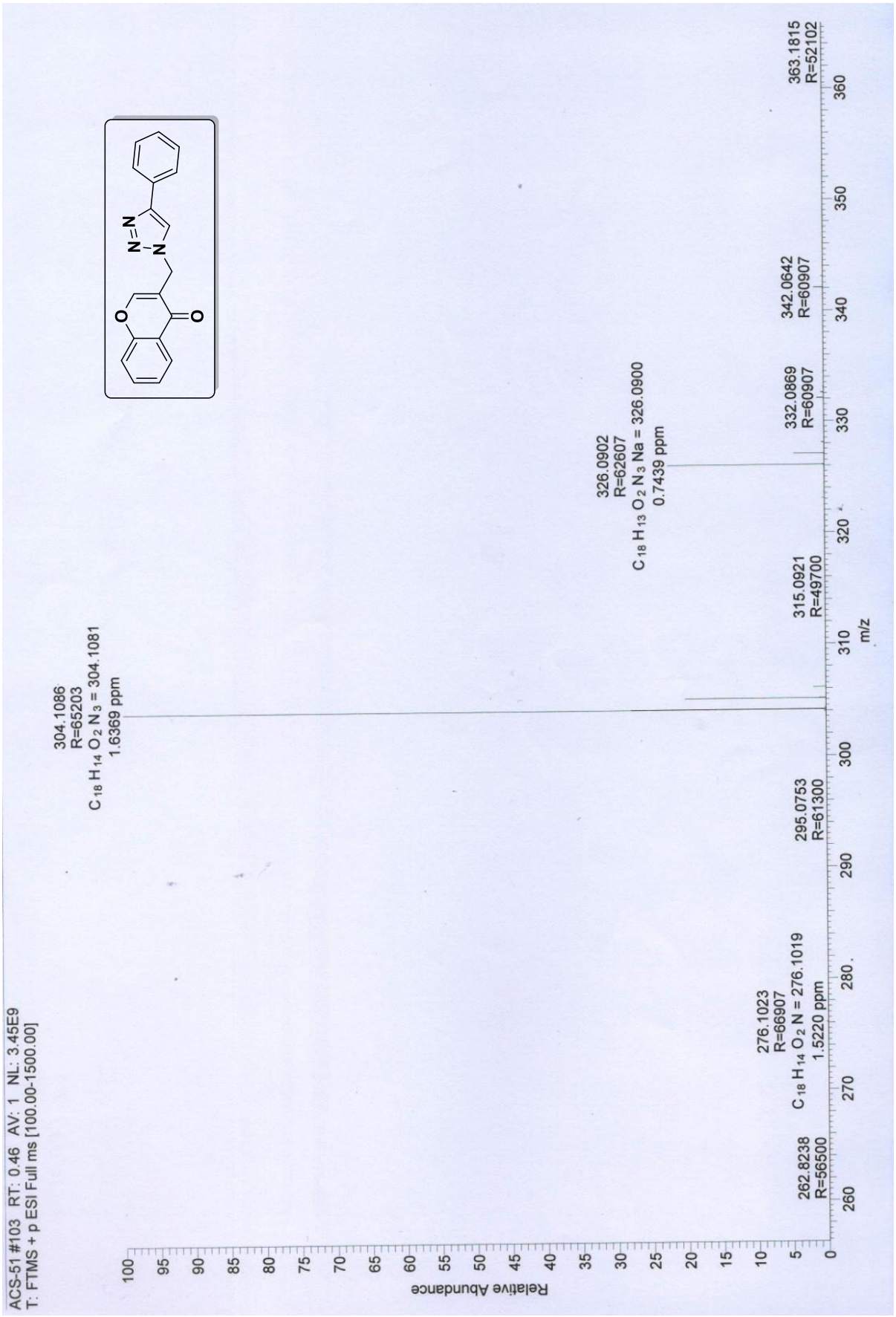
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6a***:



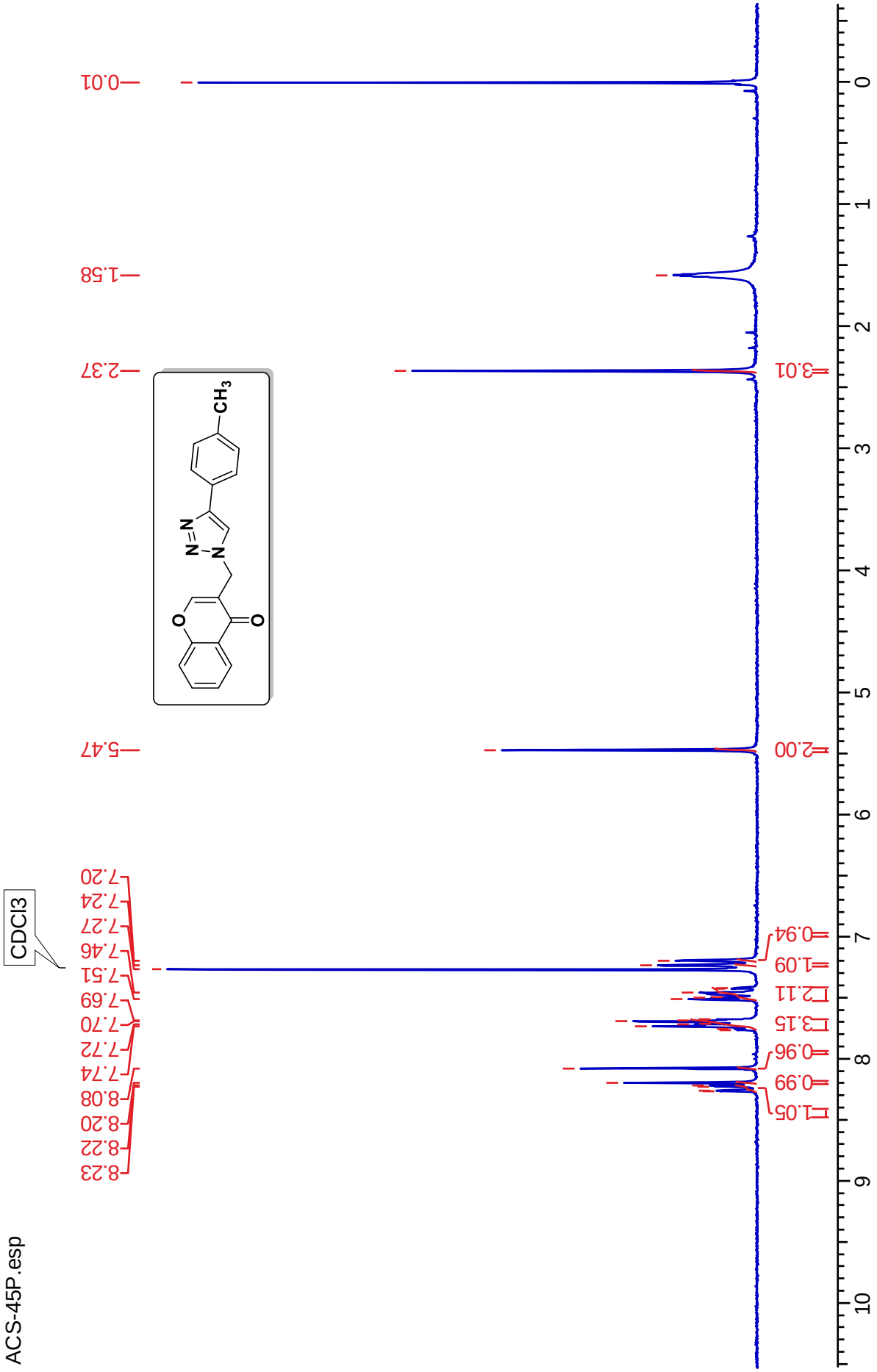
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6a***:



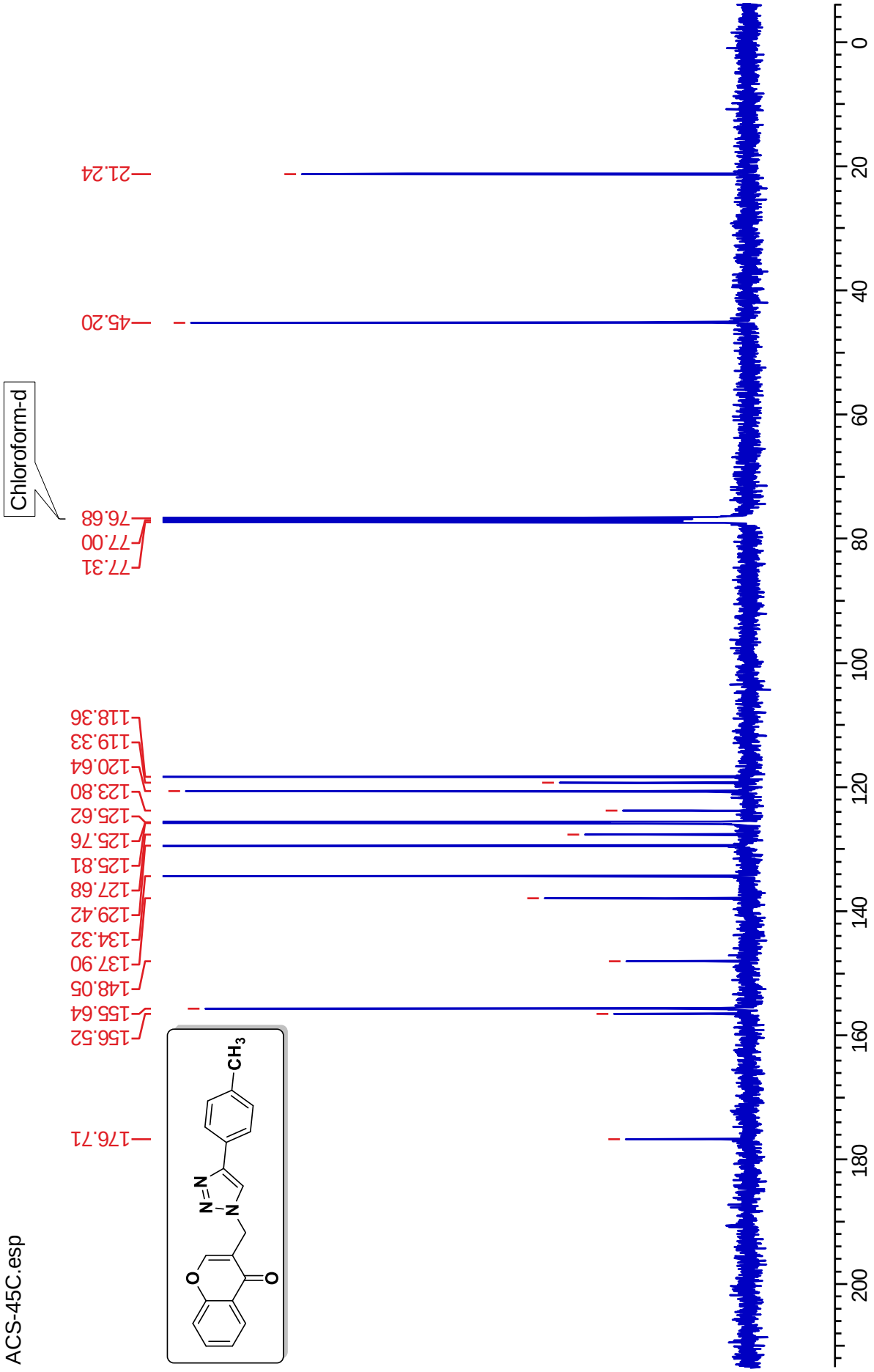
HRMS of compound ***6a***:



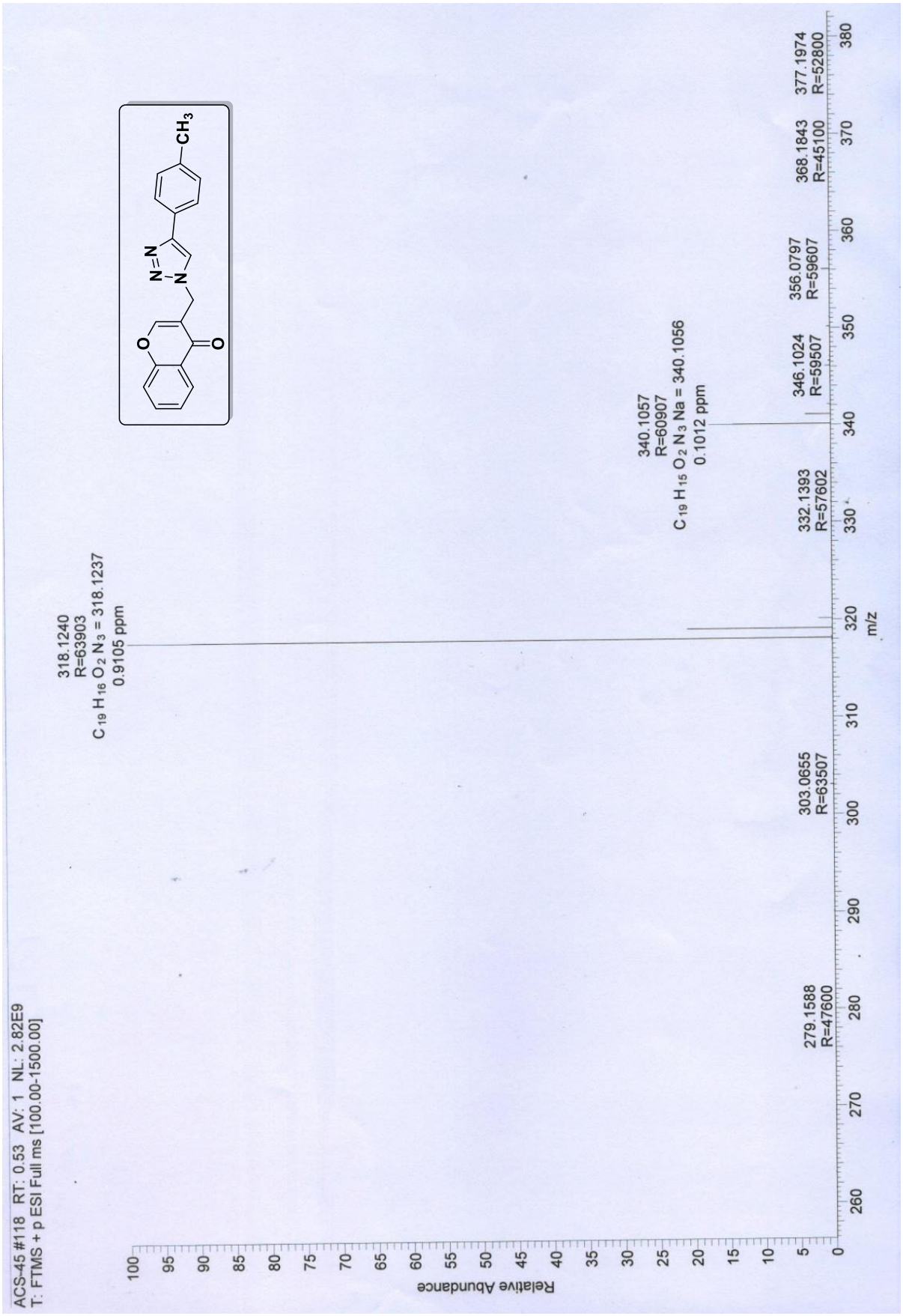
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6b***:



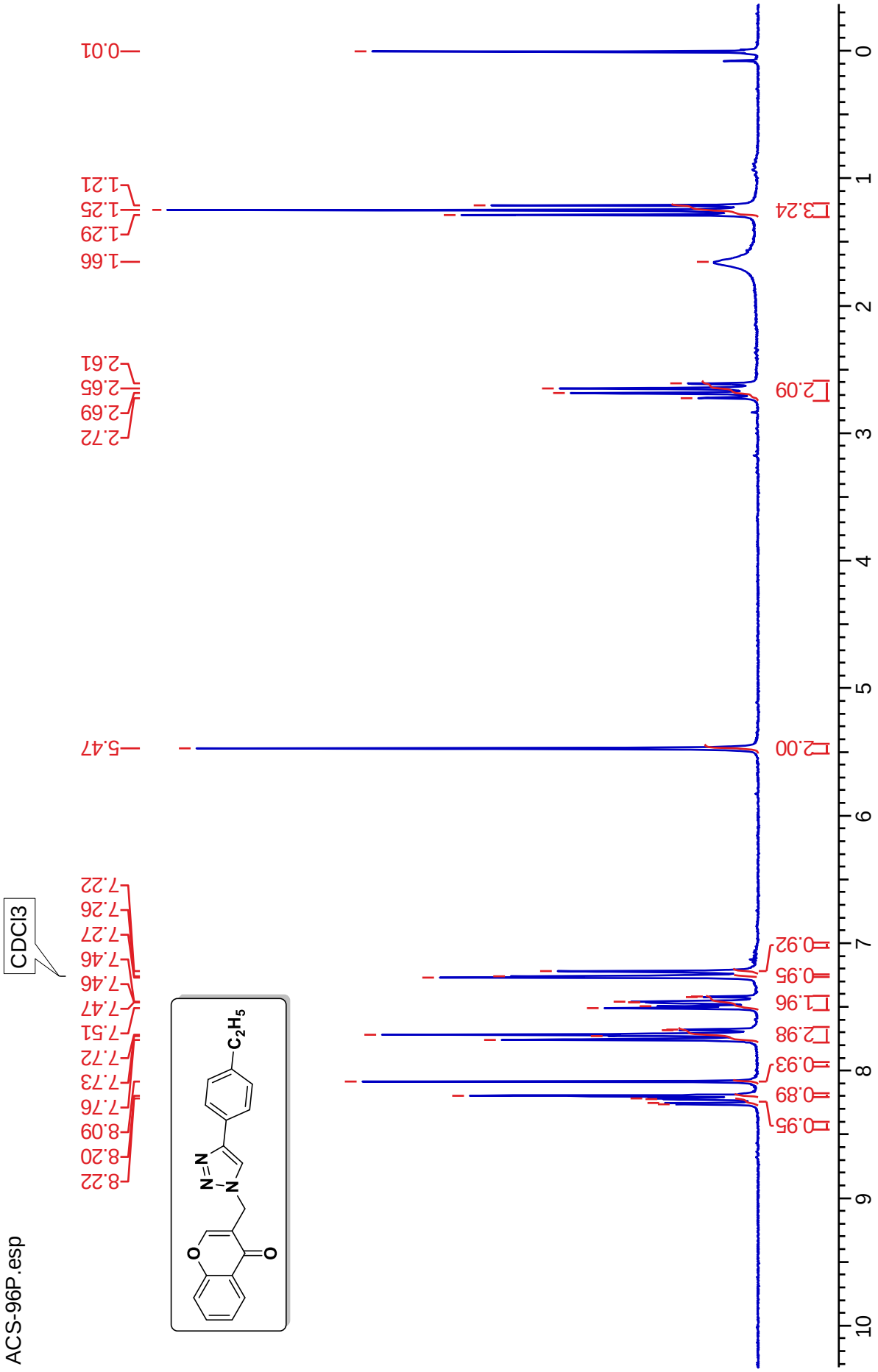
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6b***:



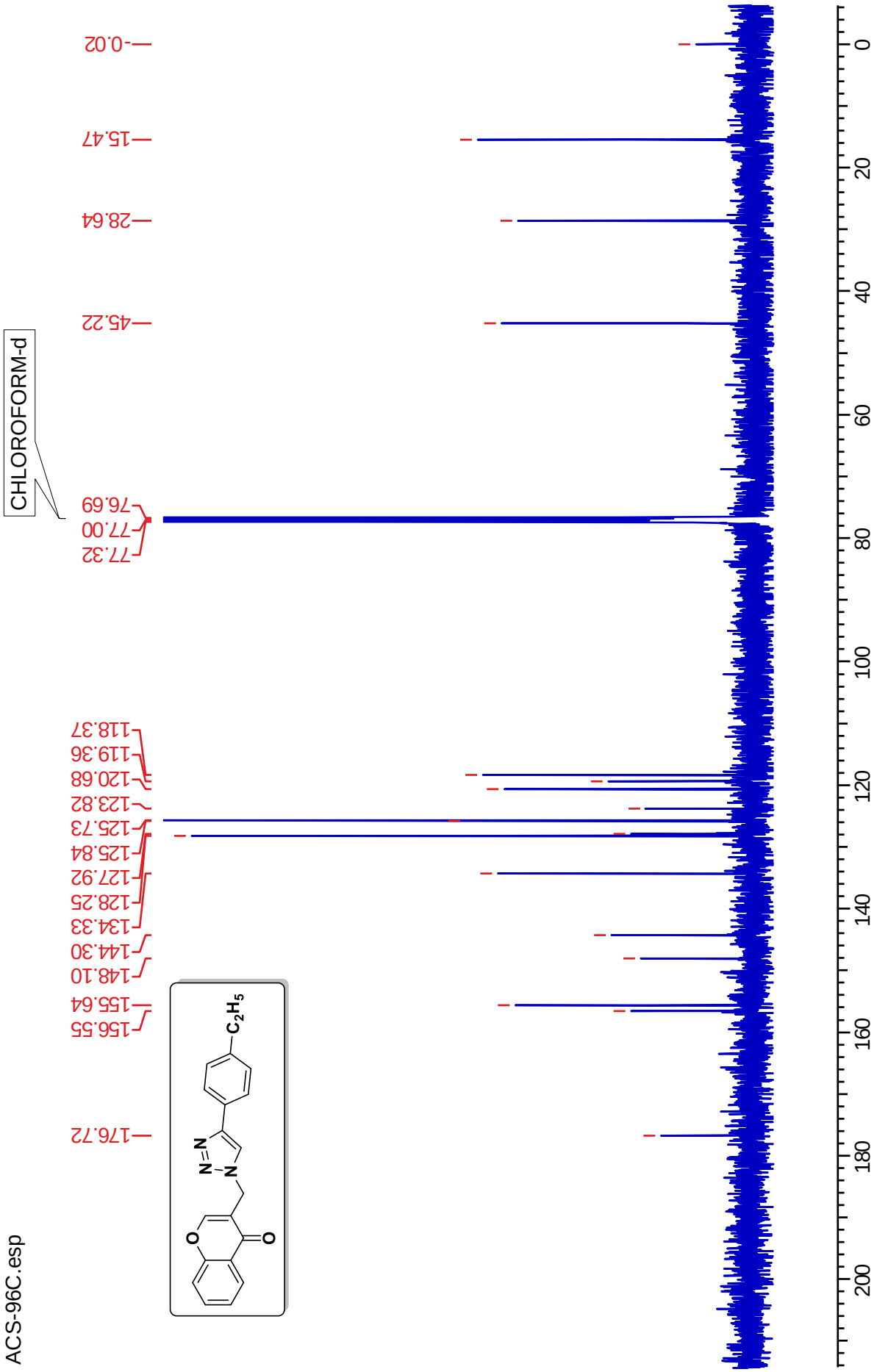
HRMS of compound ***6b***:



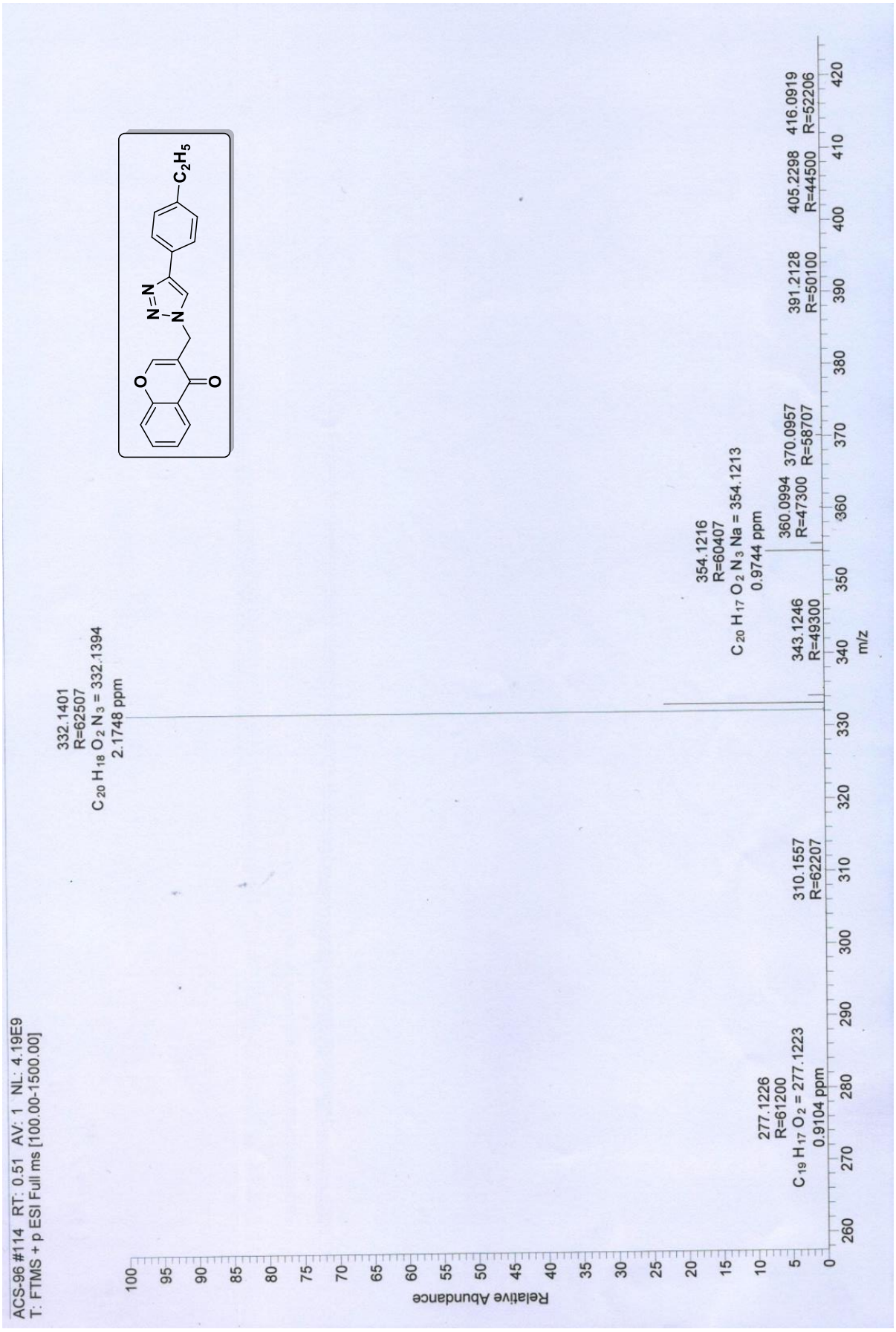
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6c***:



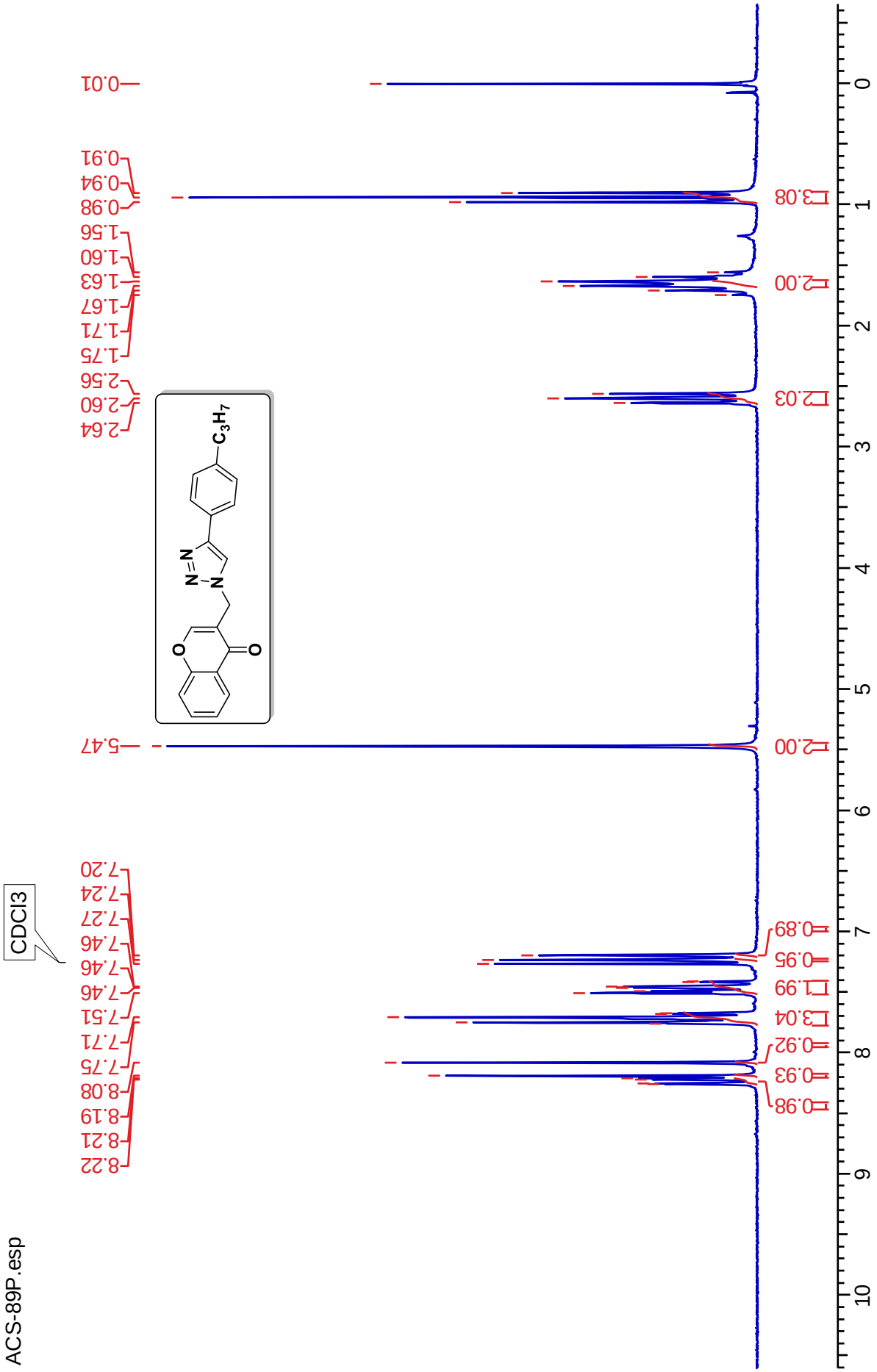
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6c***:



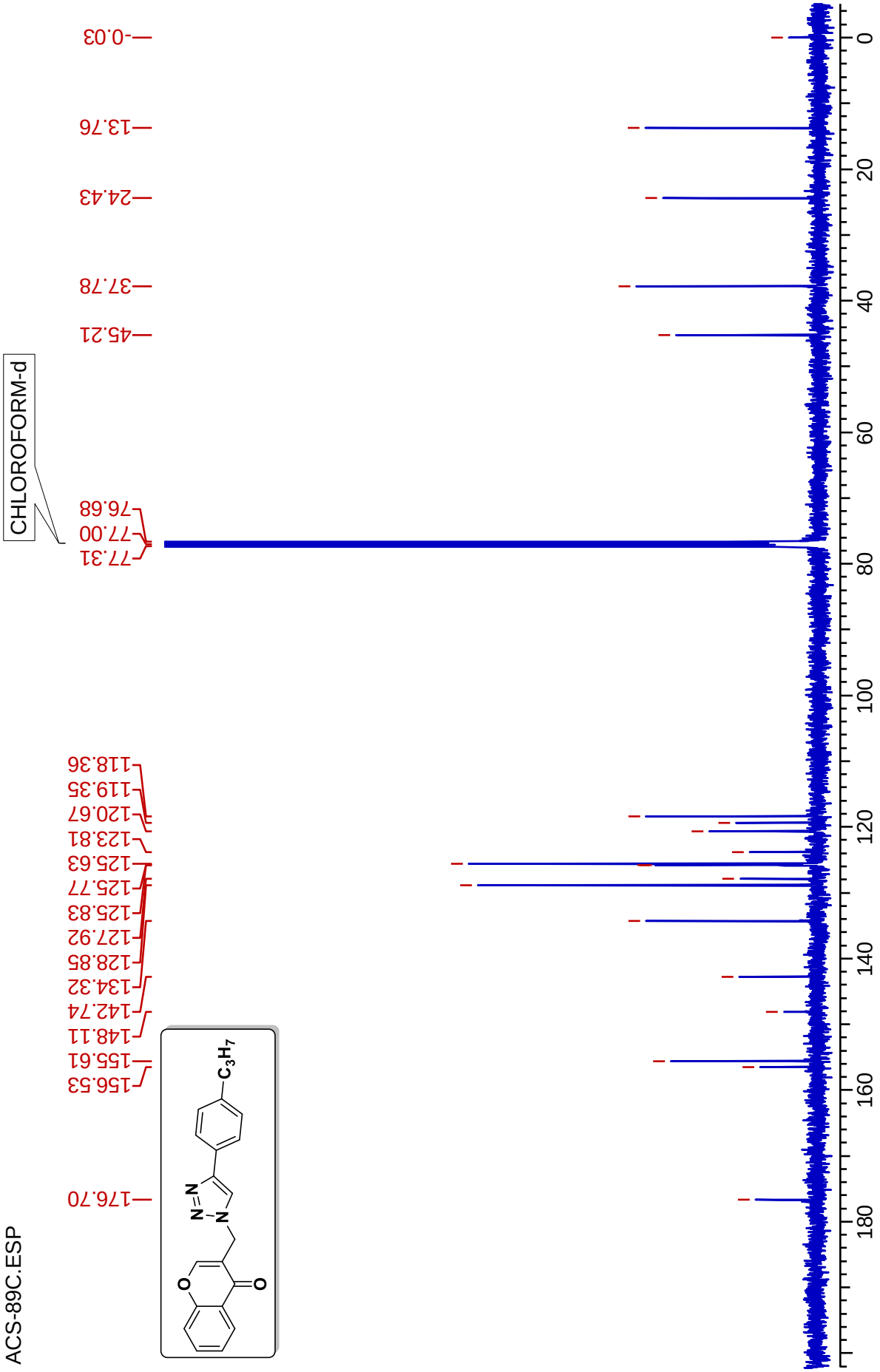
HRMS of compound ***6c***:



^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6d***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6d***:



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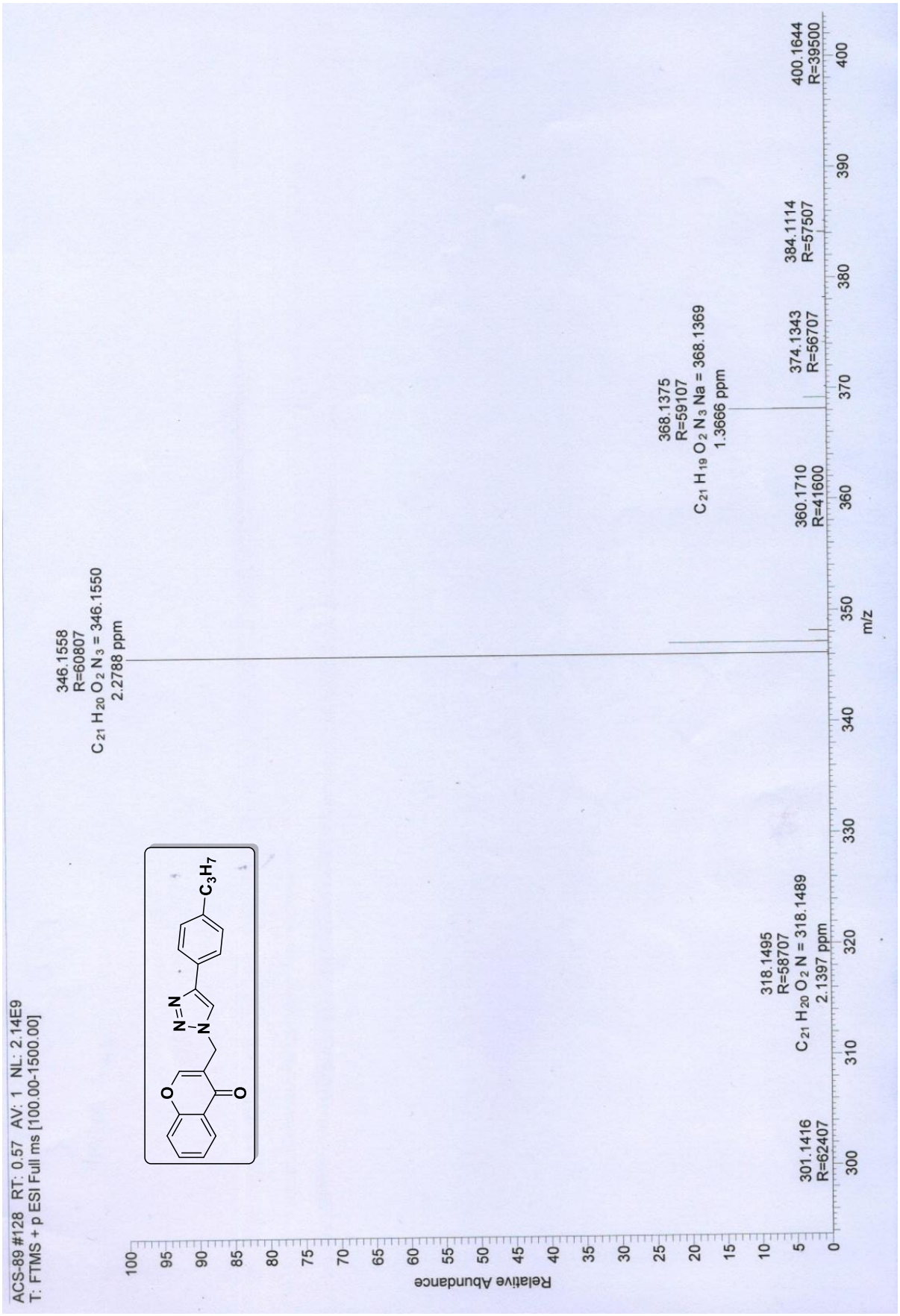
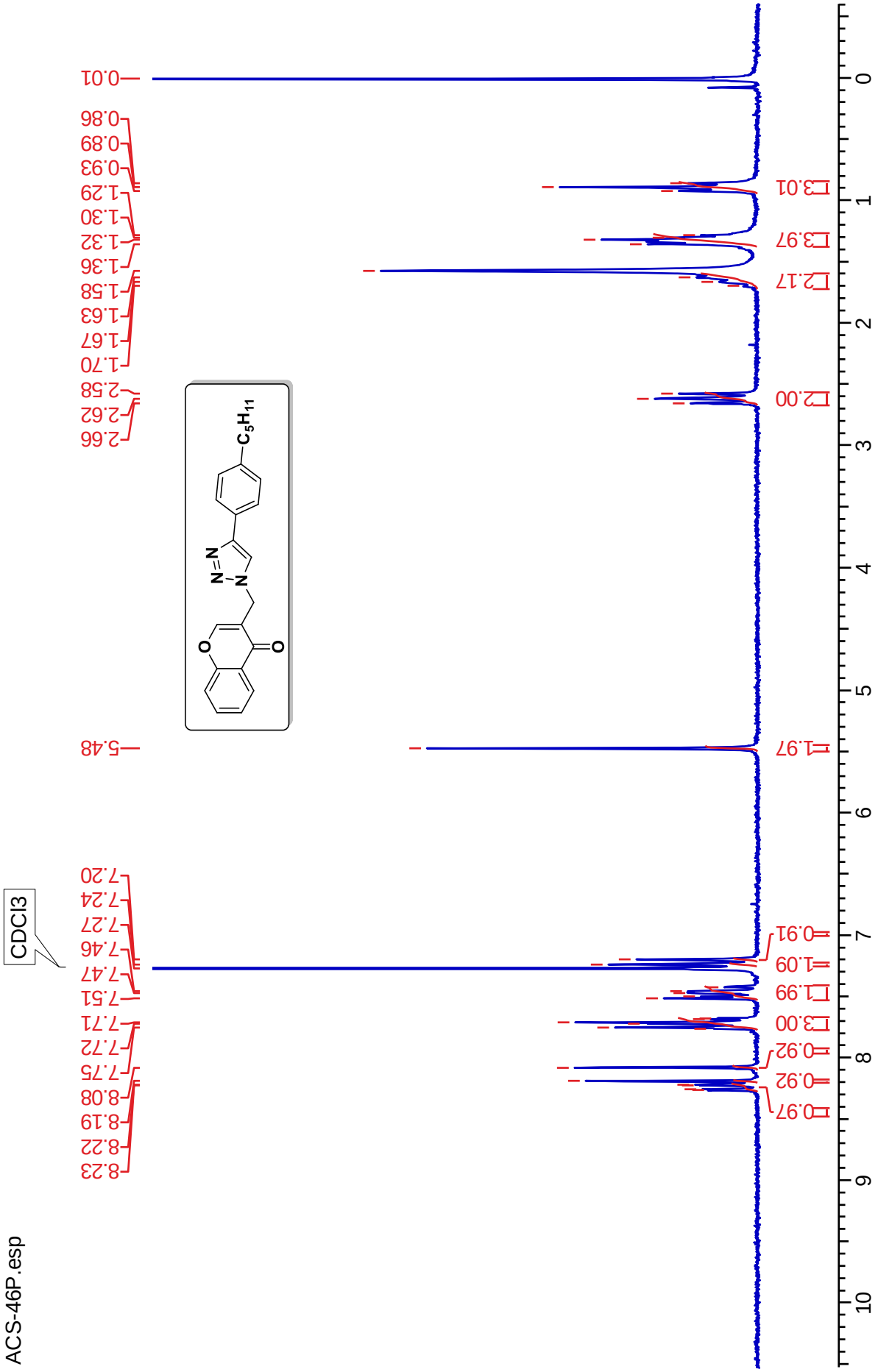
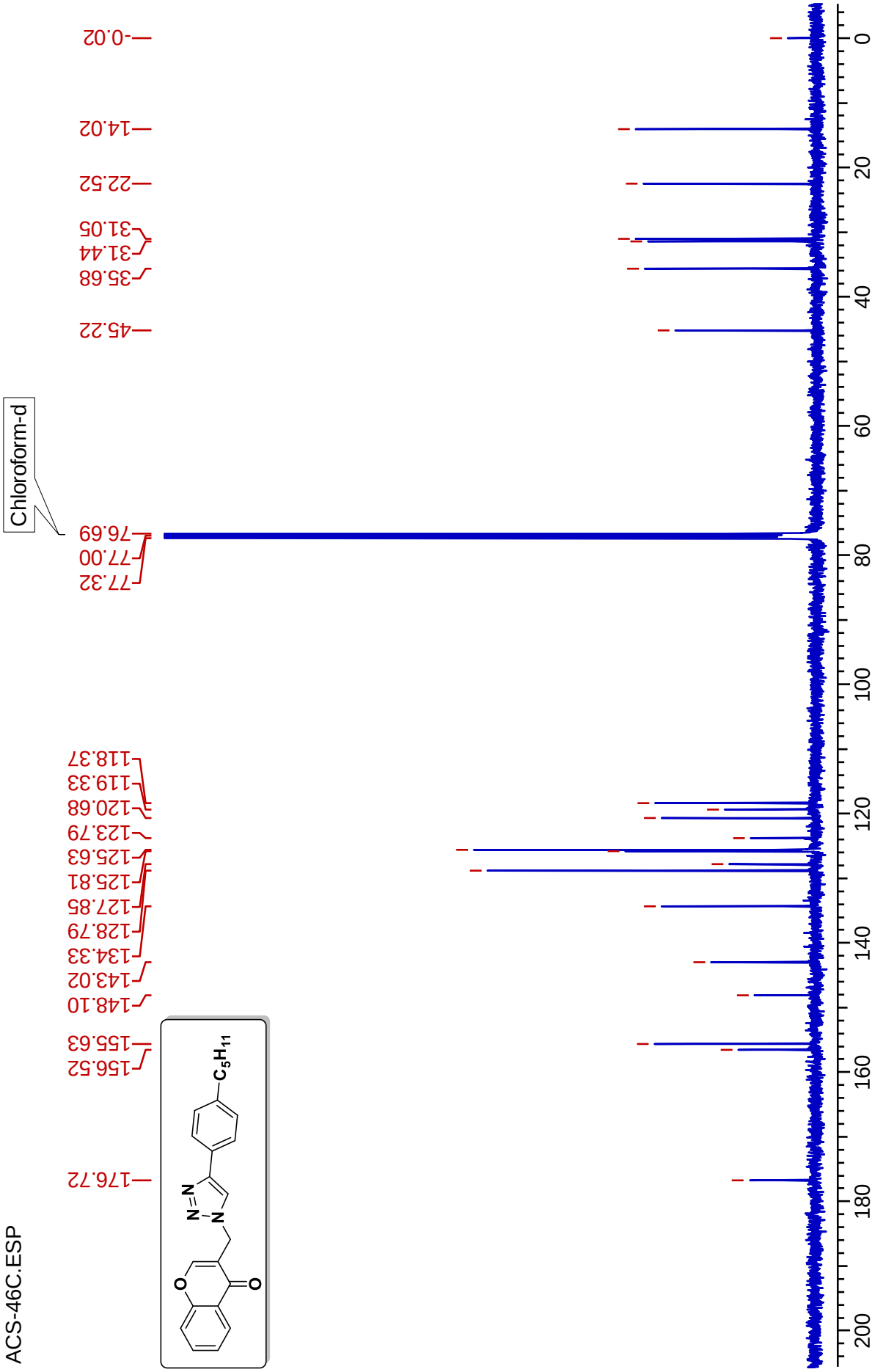


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6e***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6e***:



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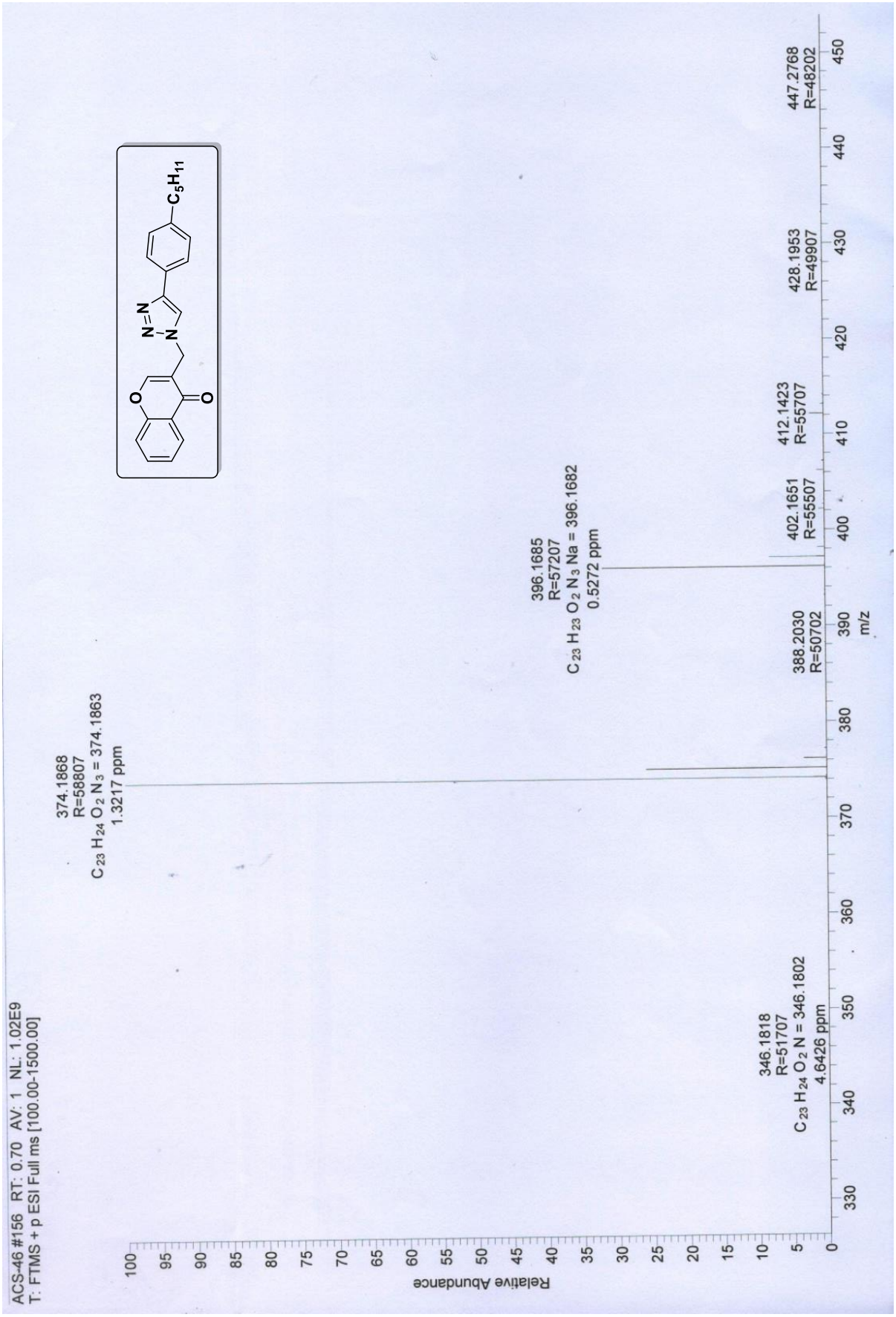
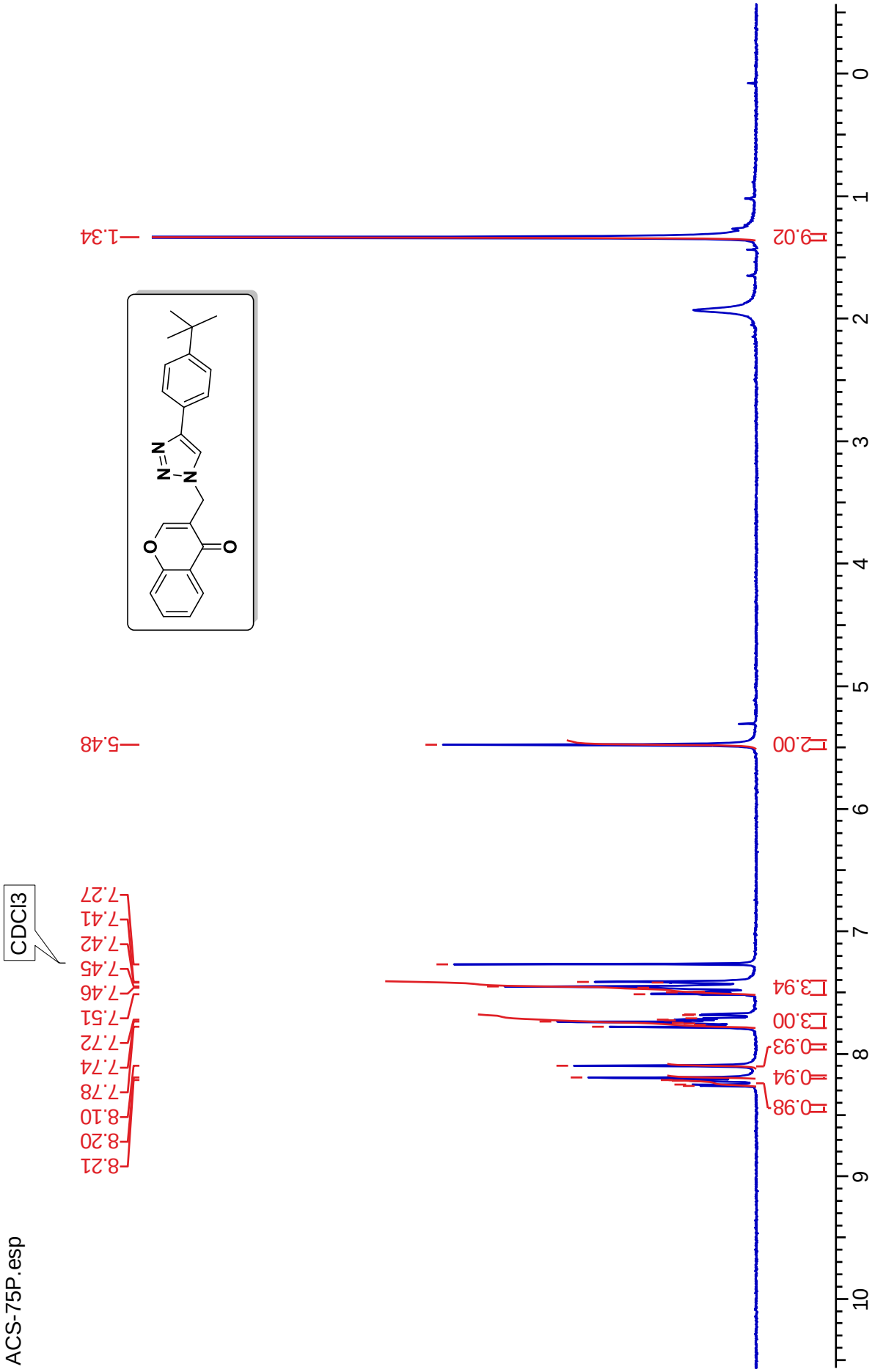
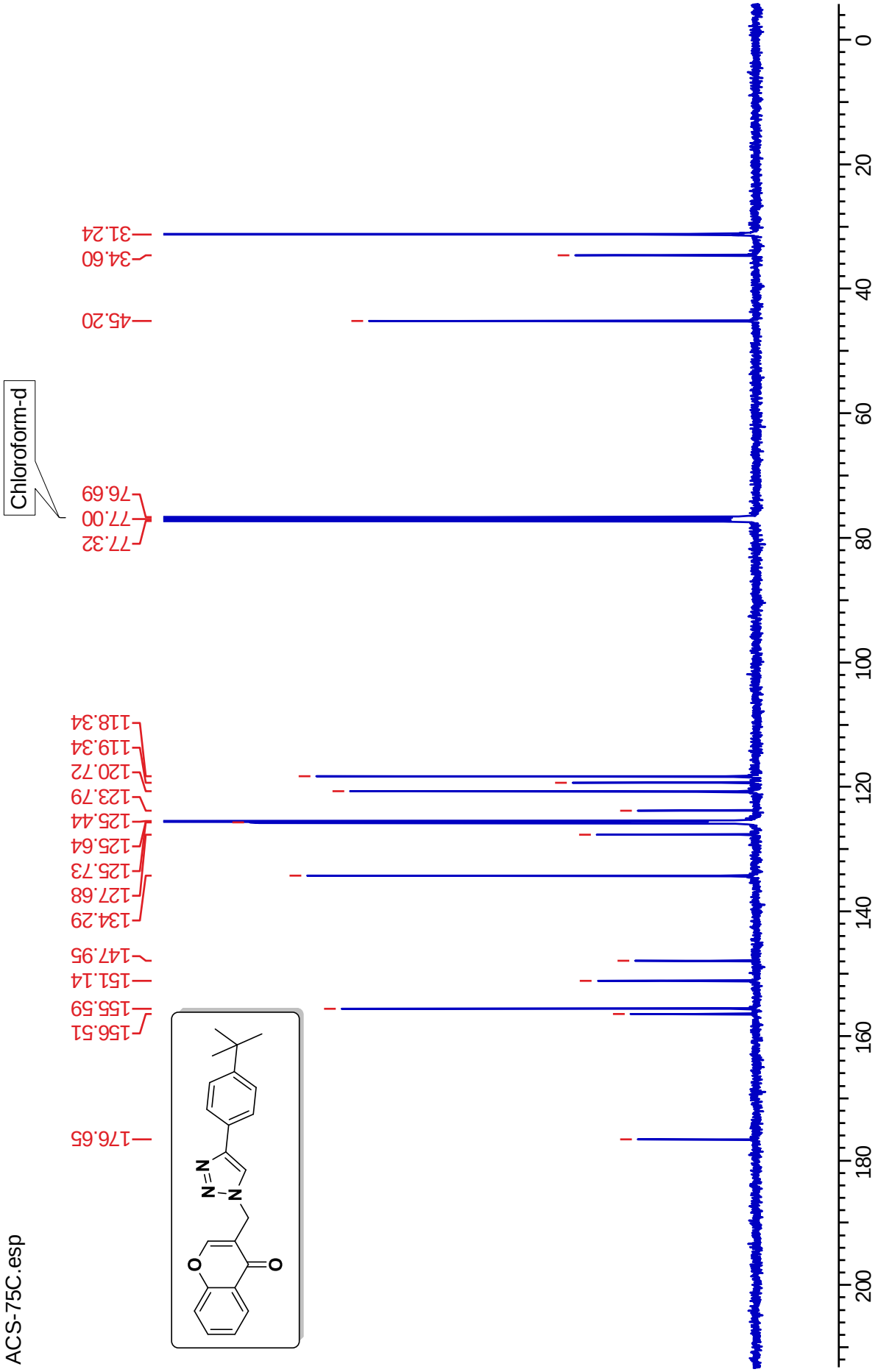


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6f***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6f***:



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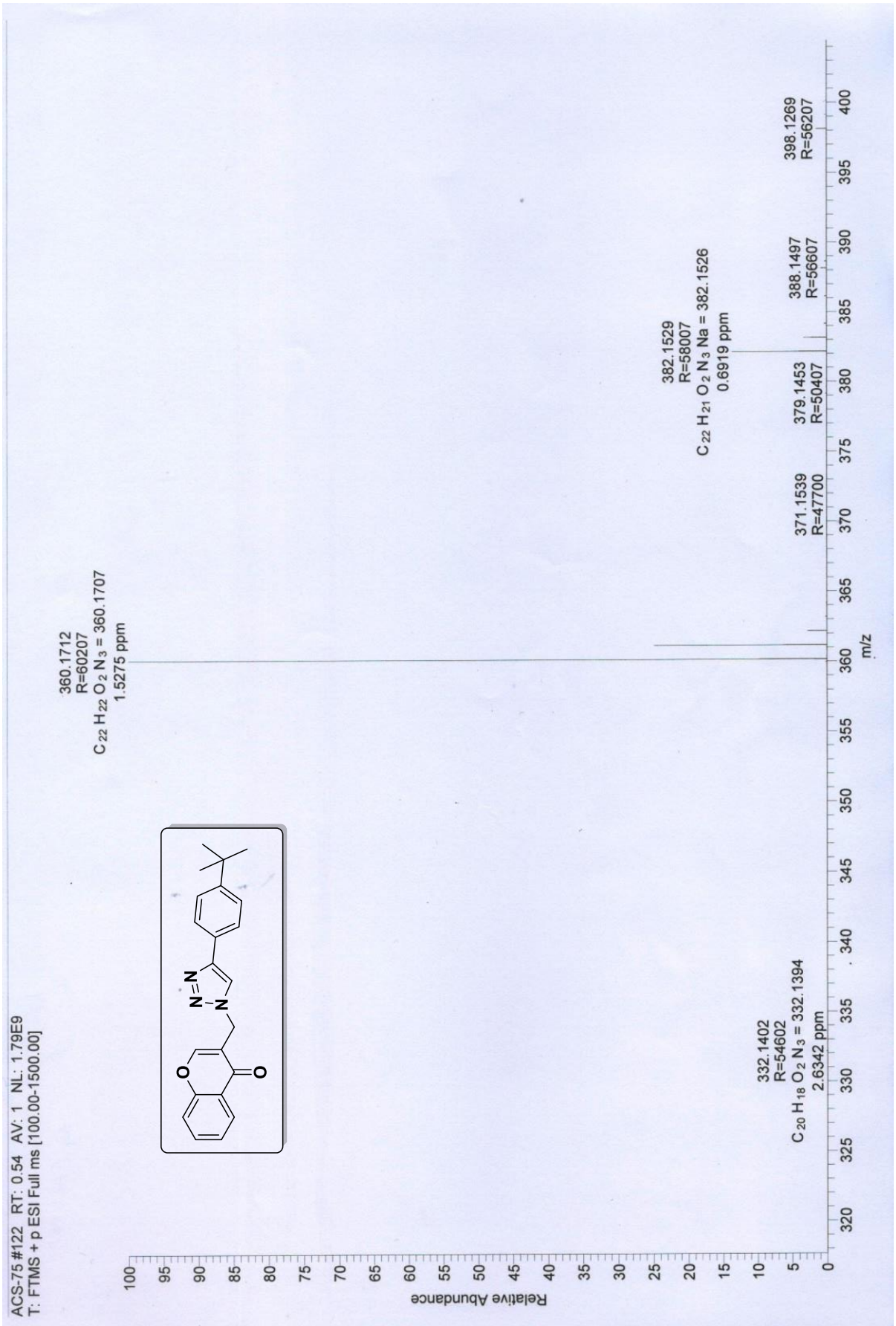
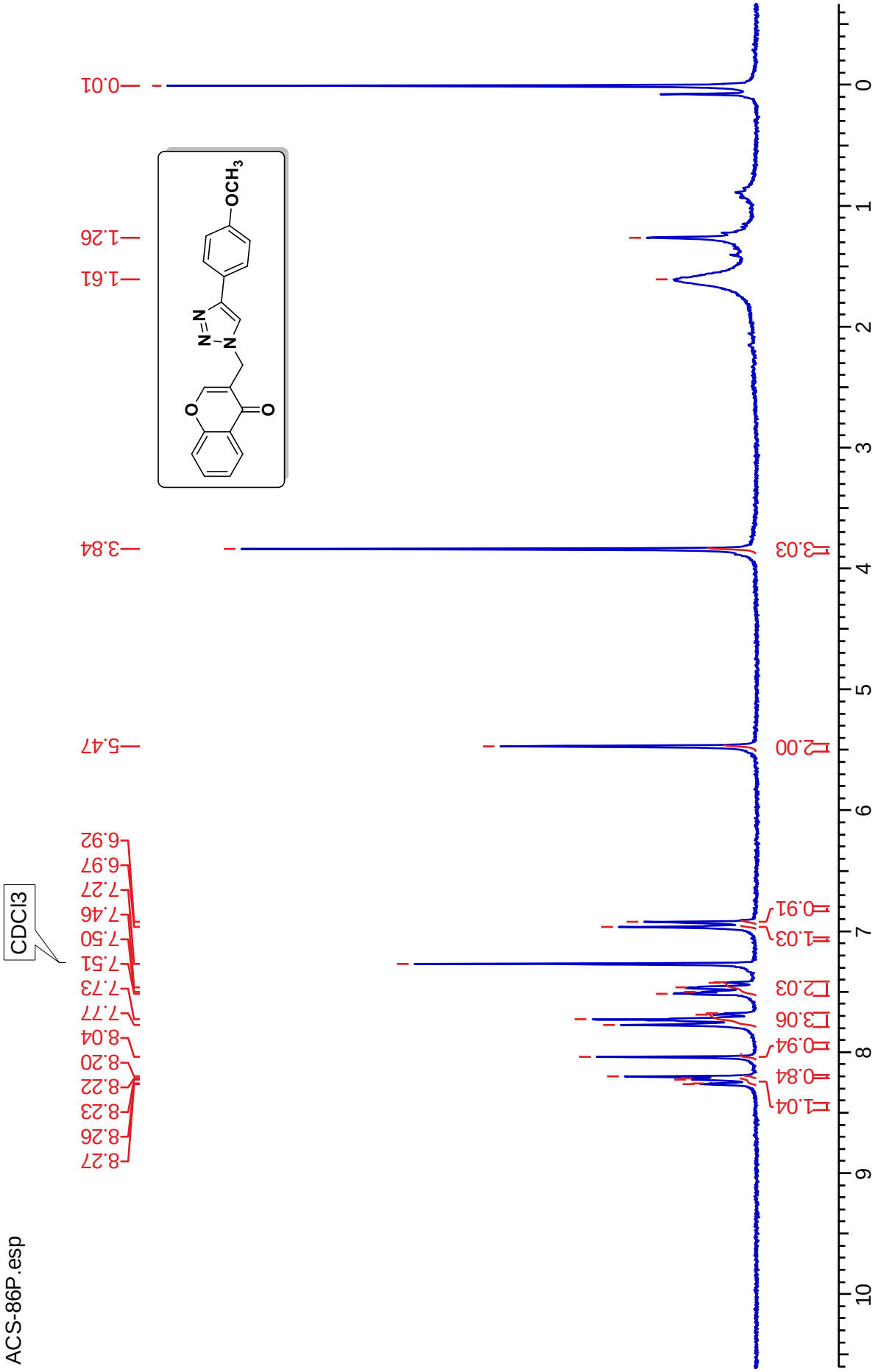
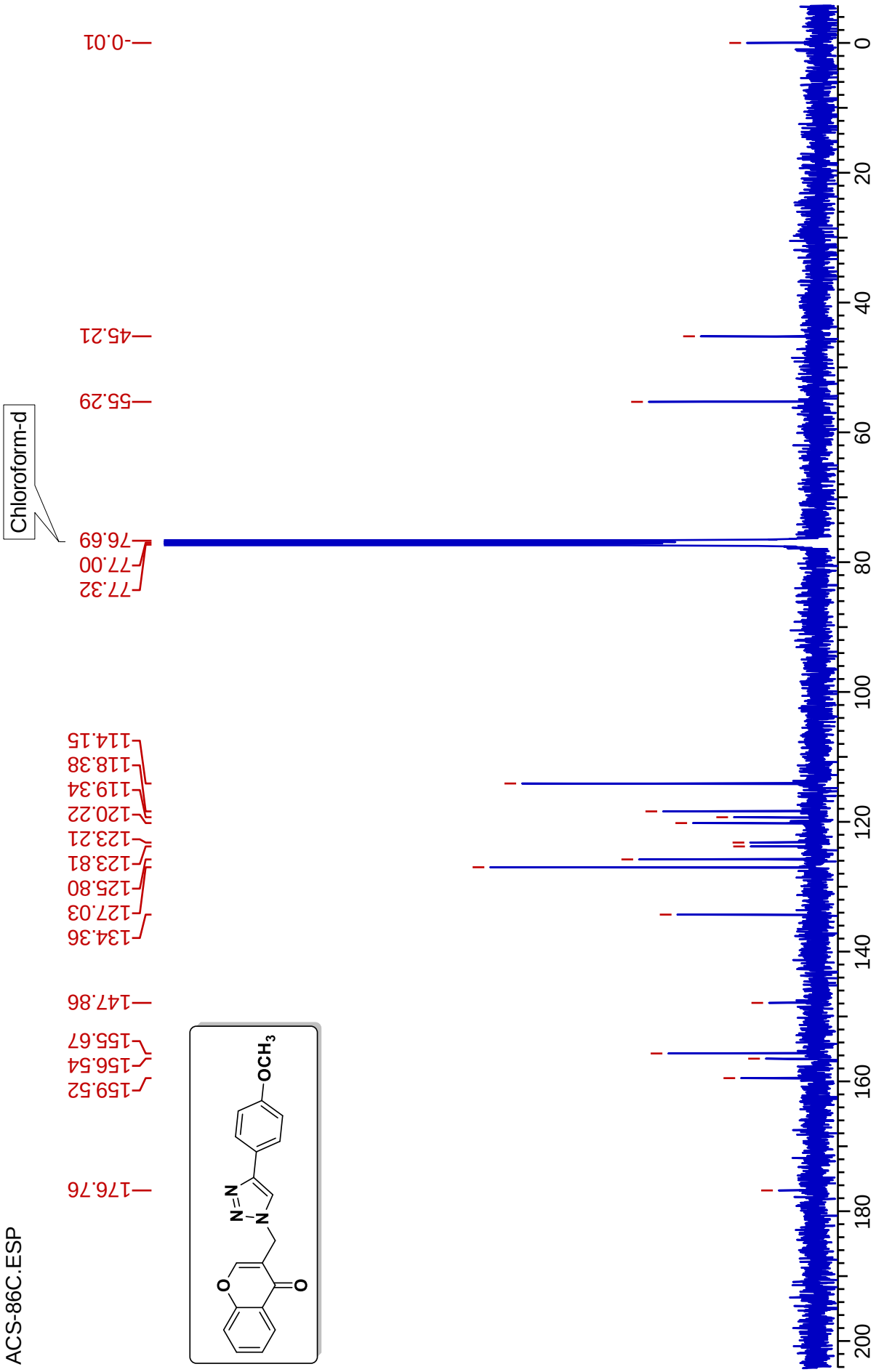


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6g***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6g***:



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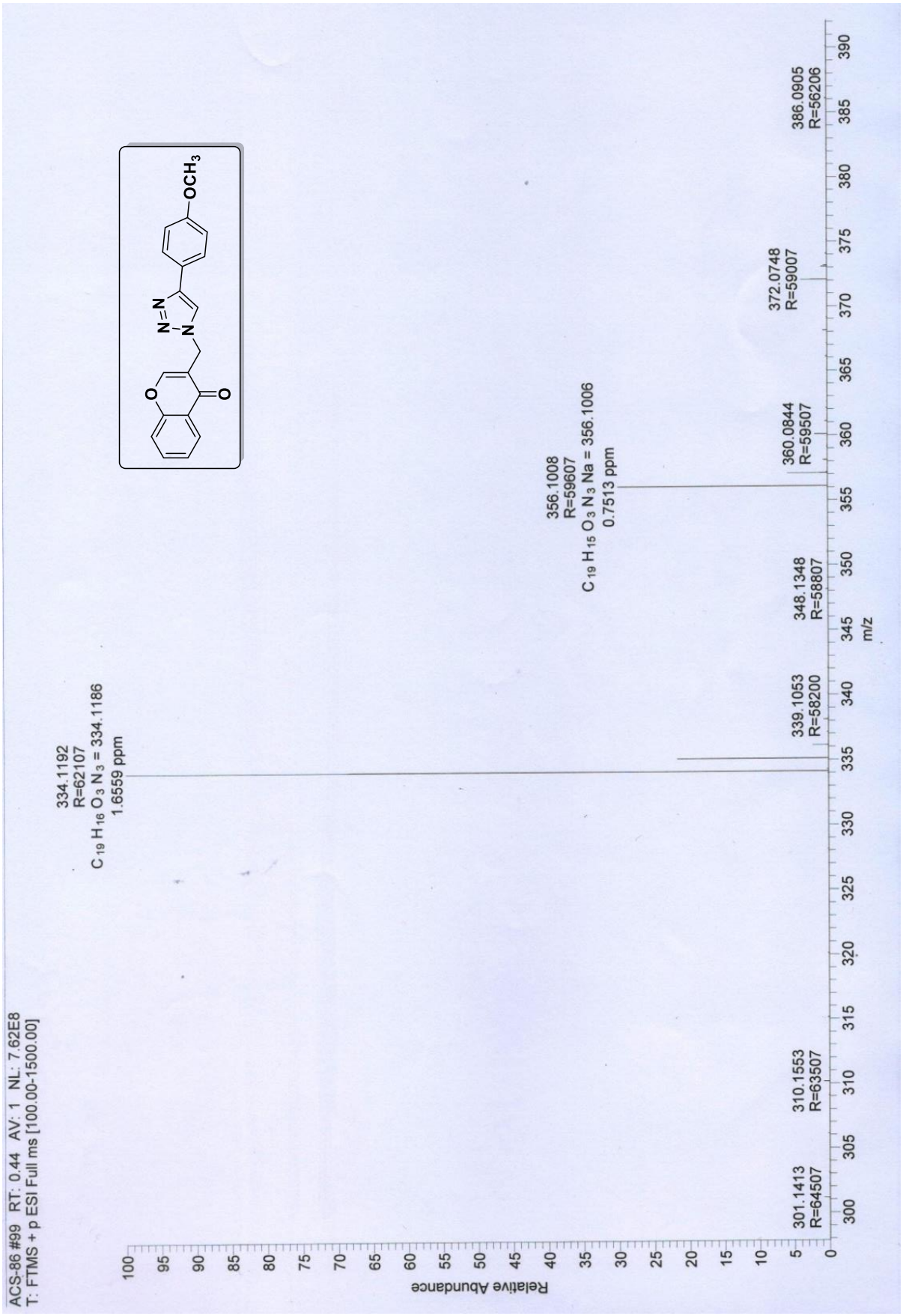
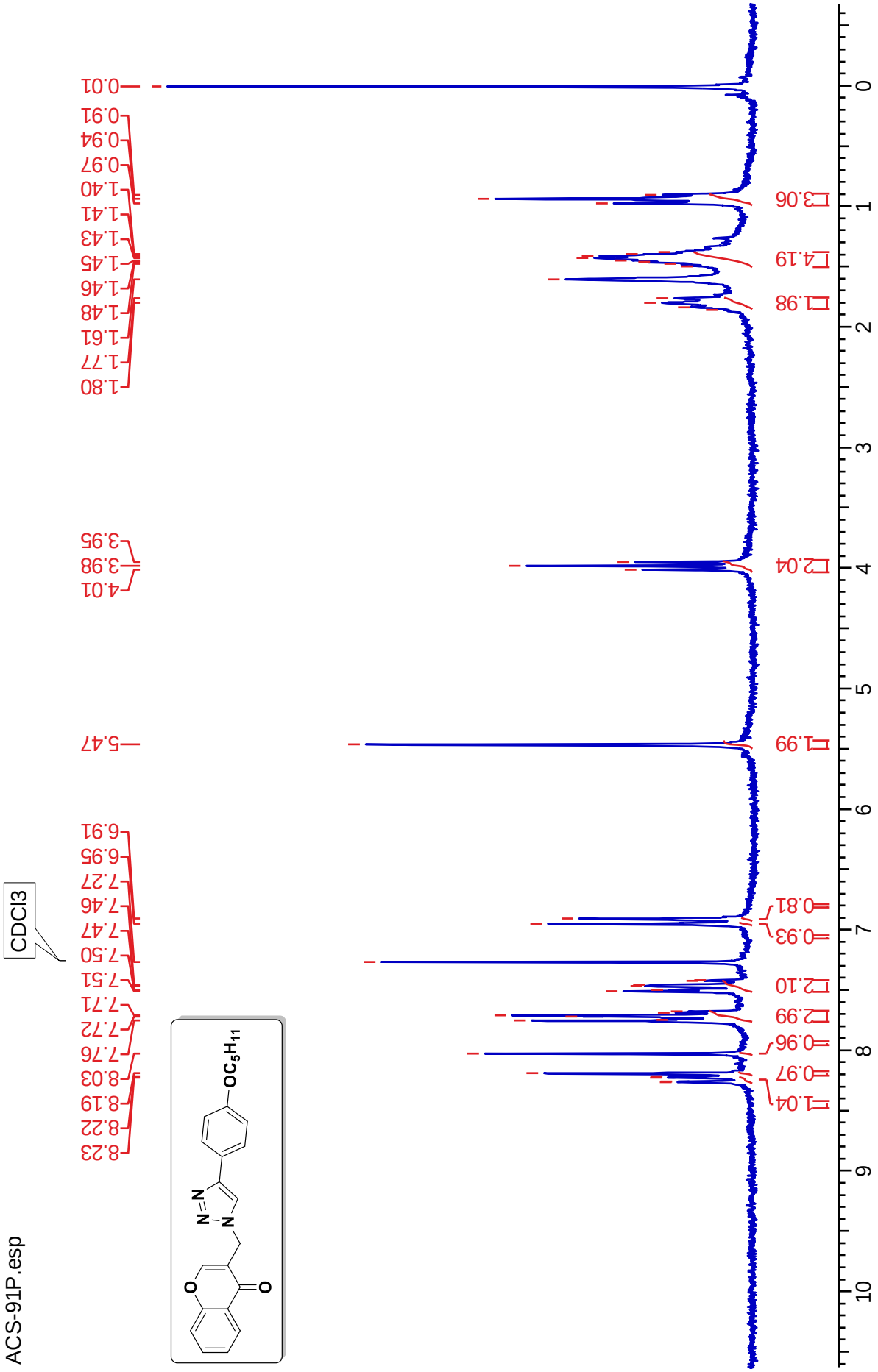
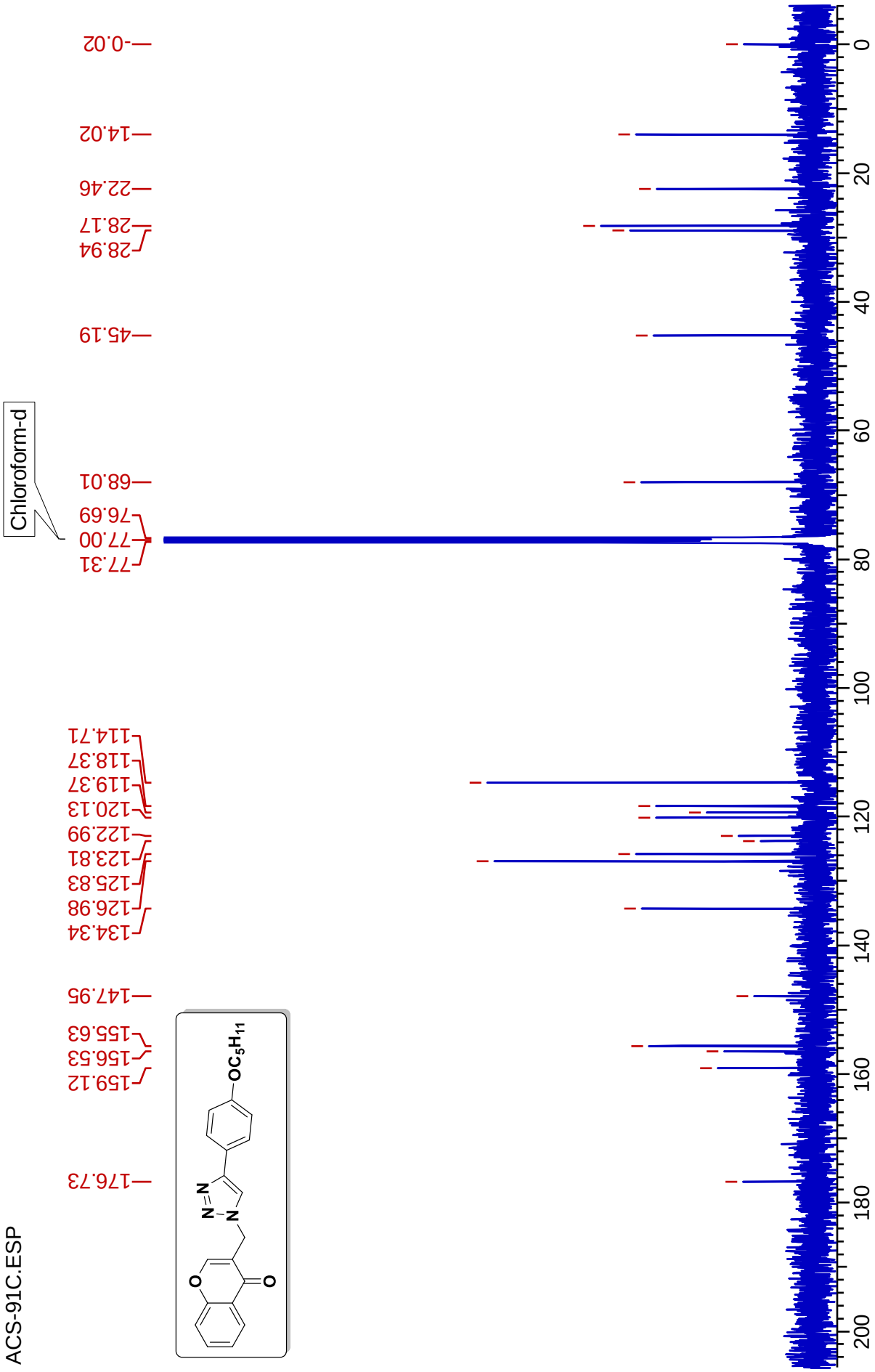


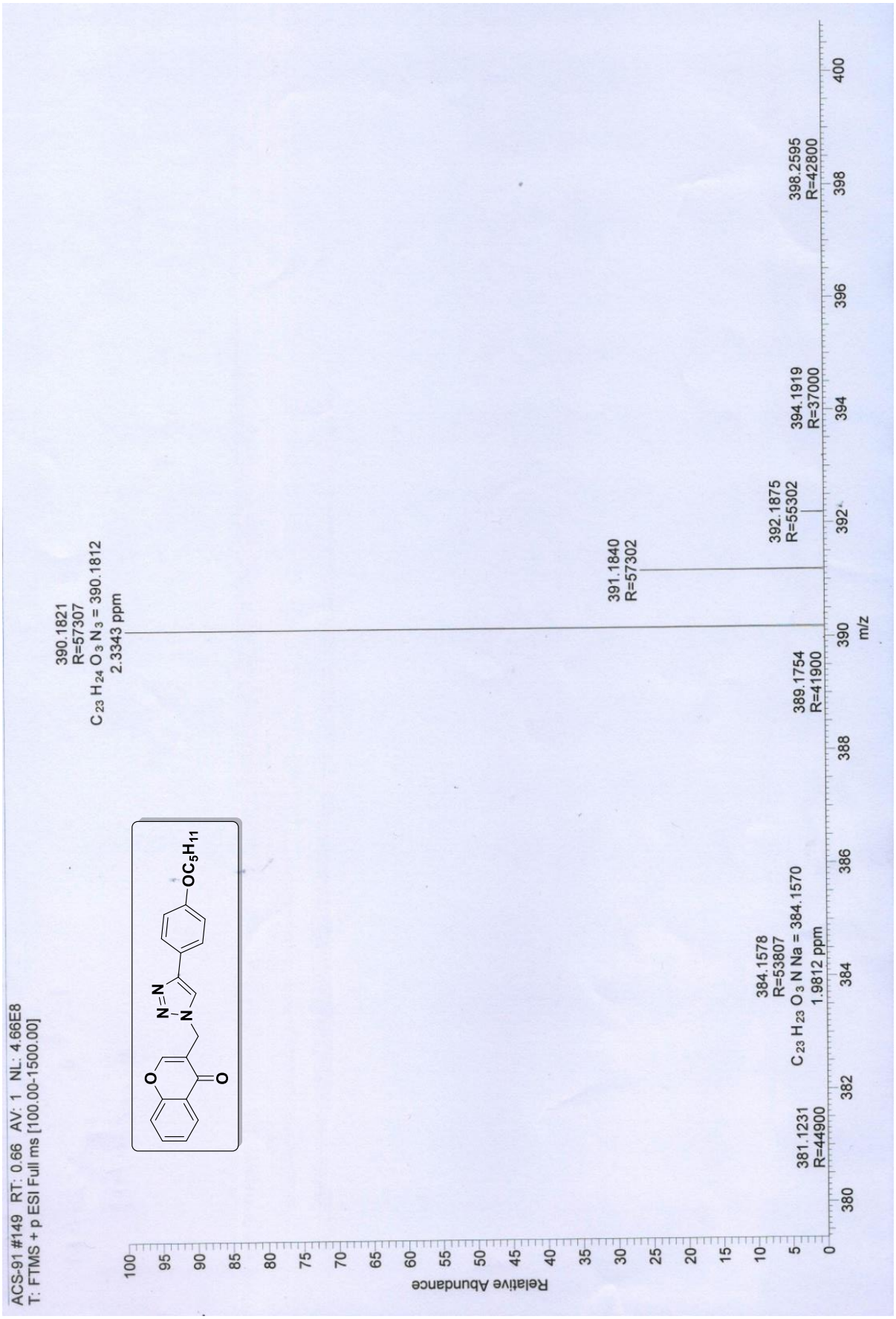
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6h***:



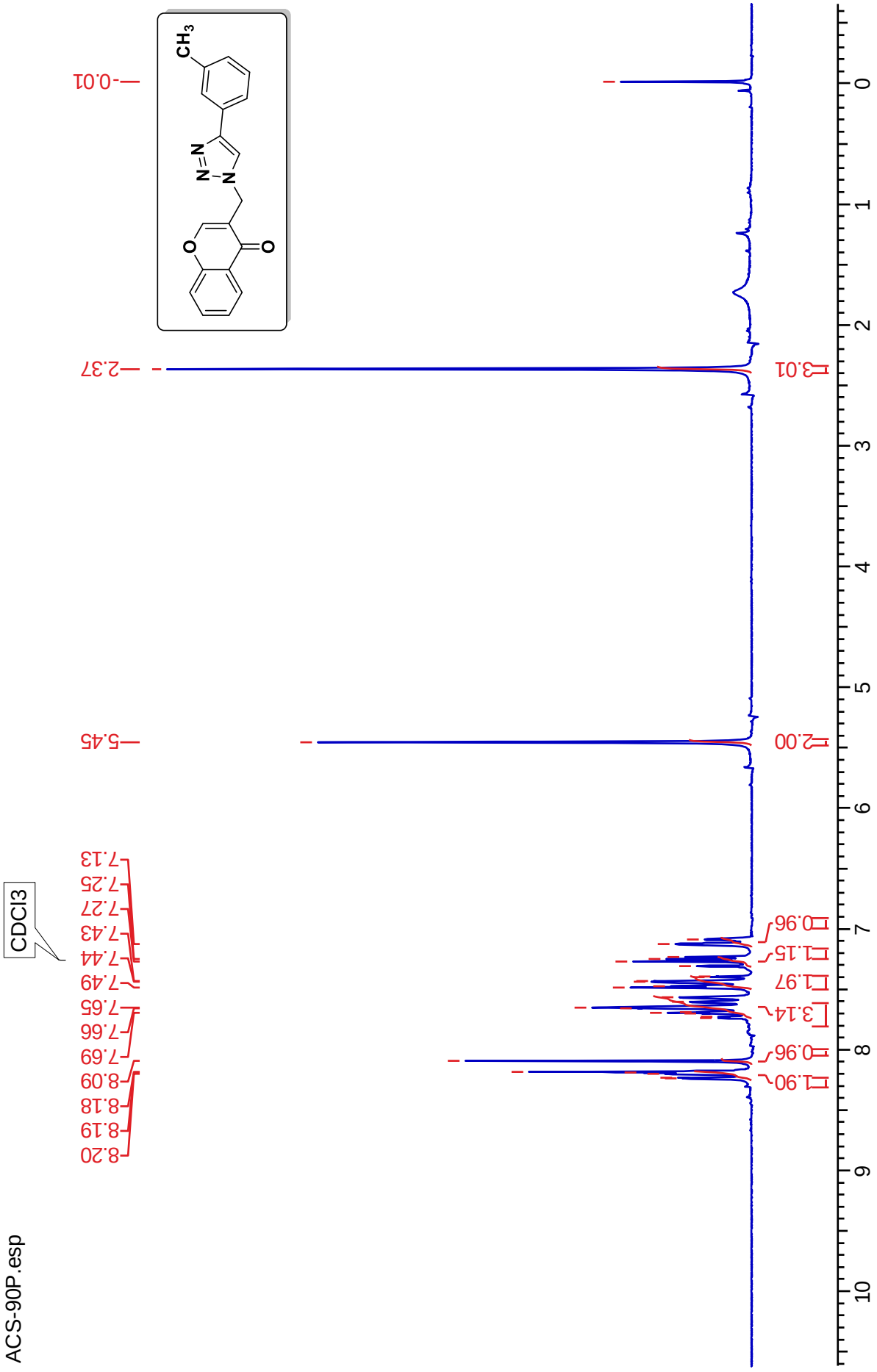
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6h***:



HRMS of compound ***6h***:



^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6i***:



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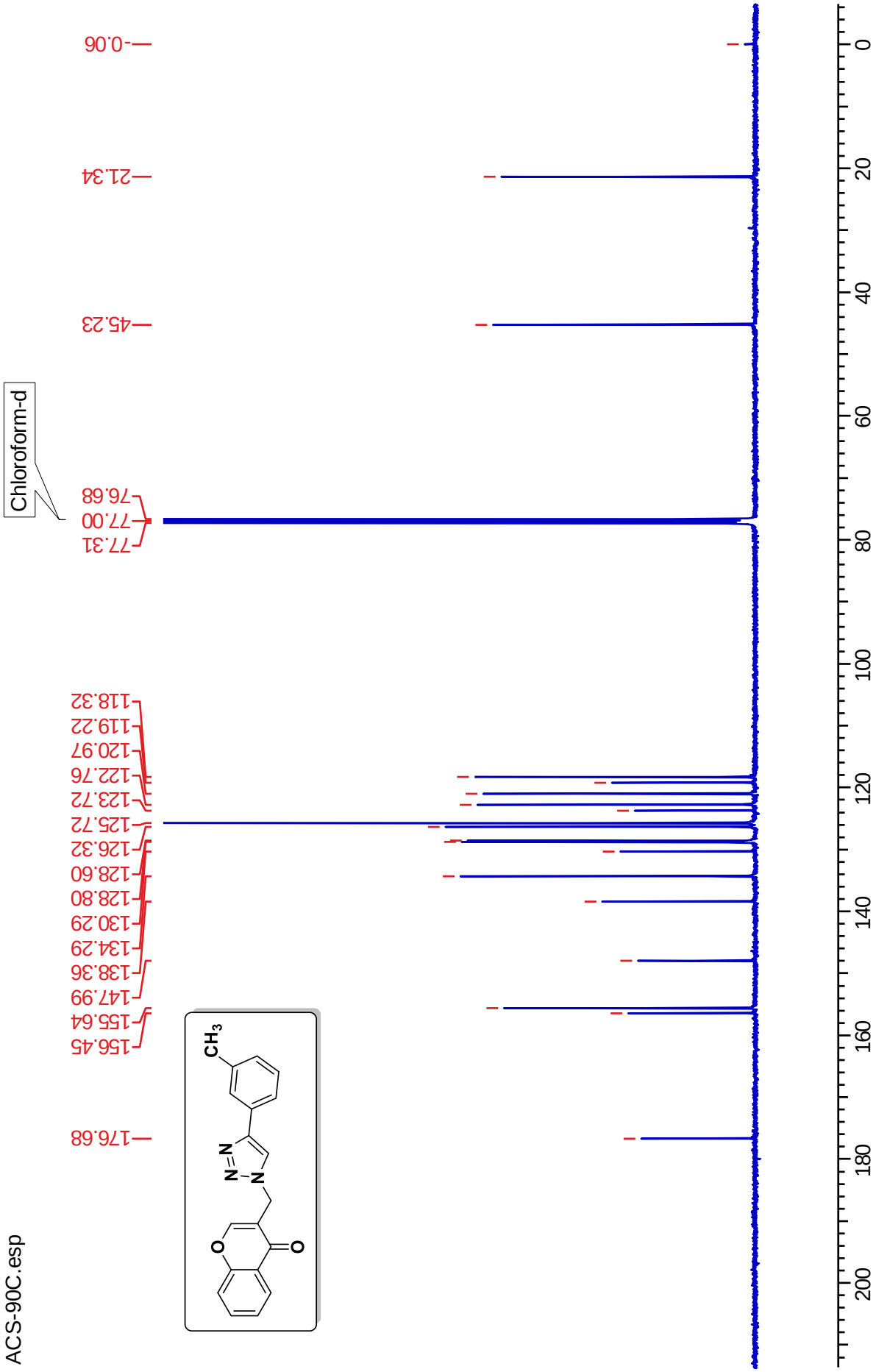

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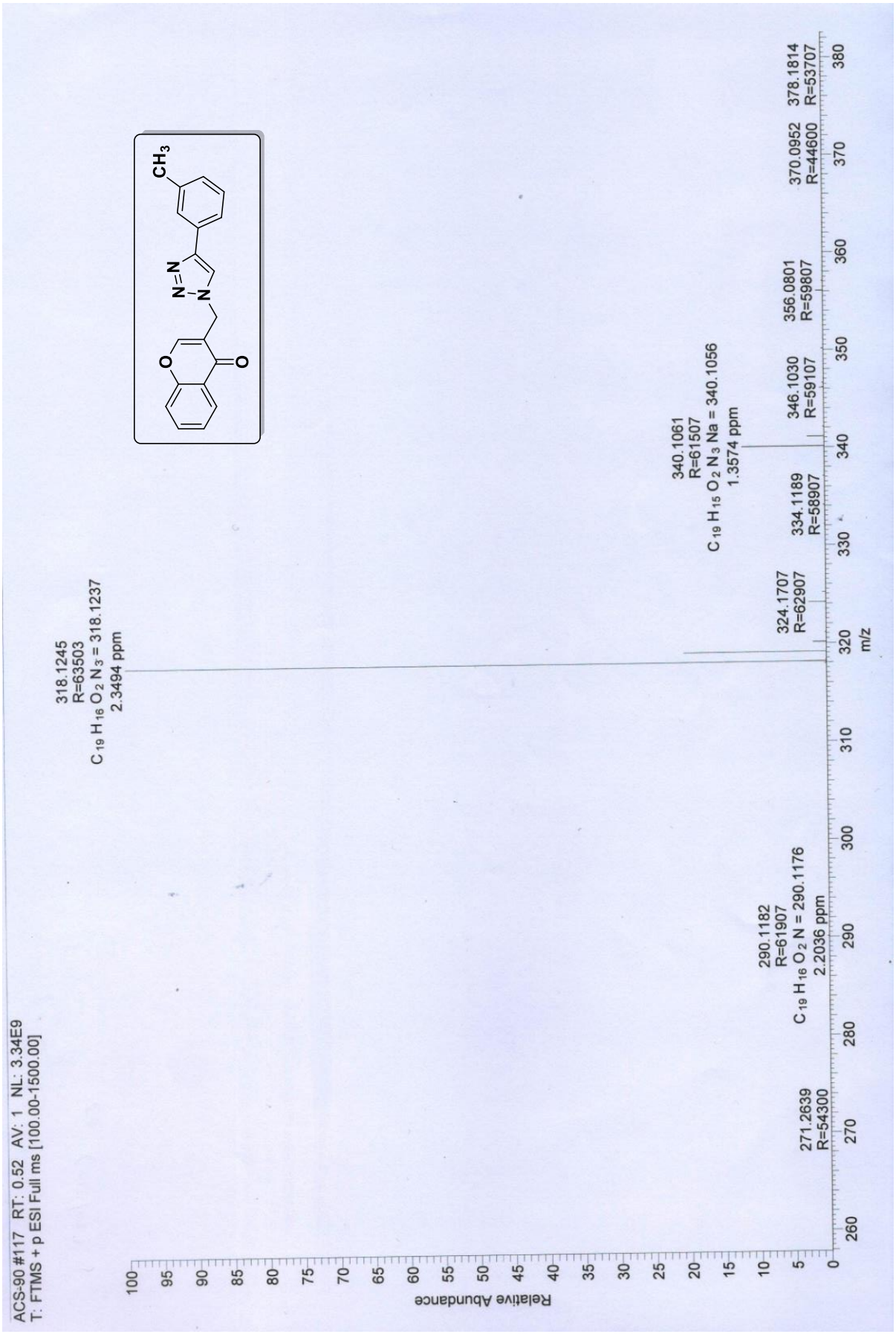
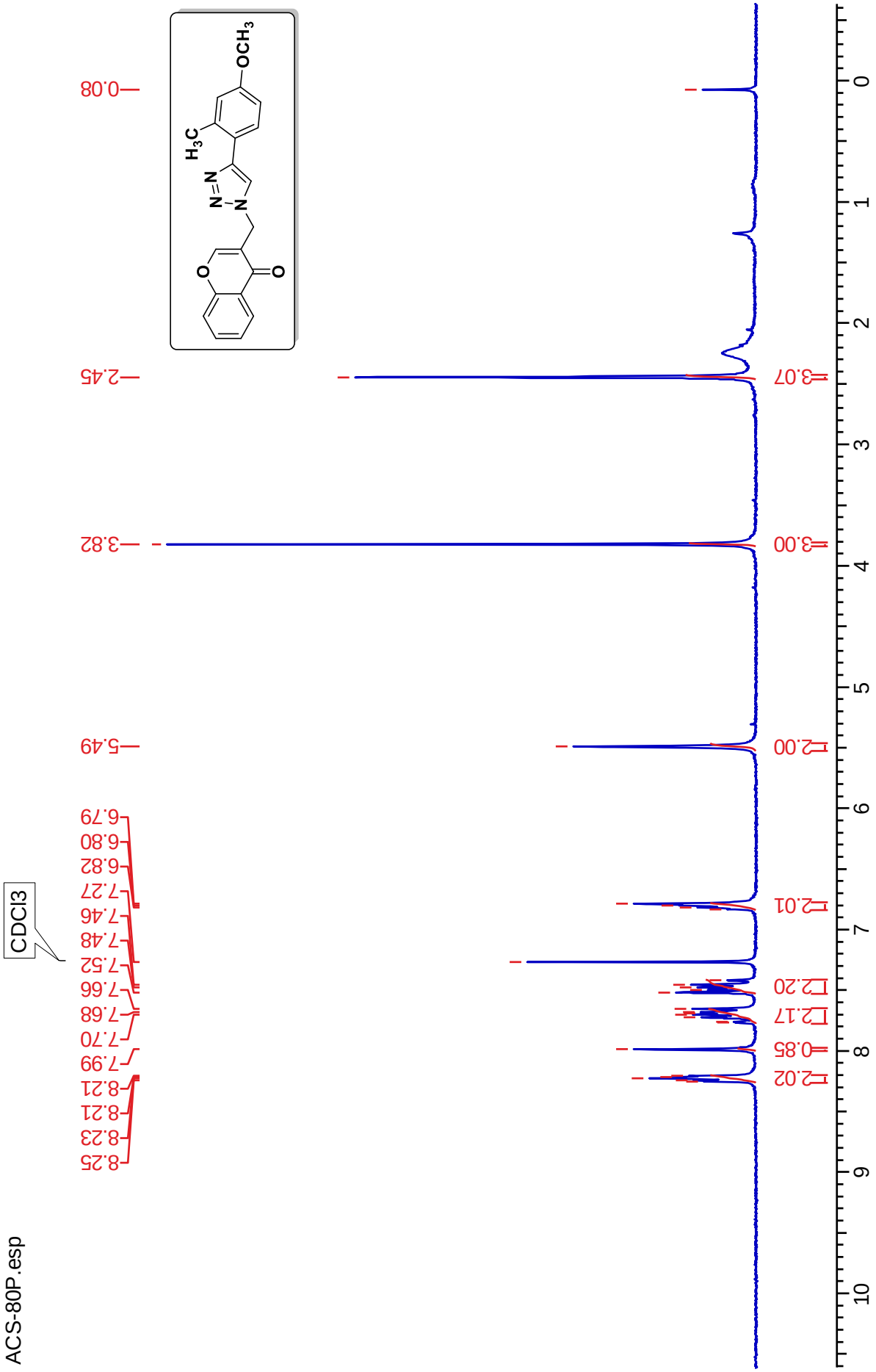


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6j***:



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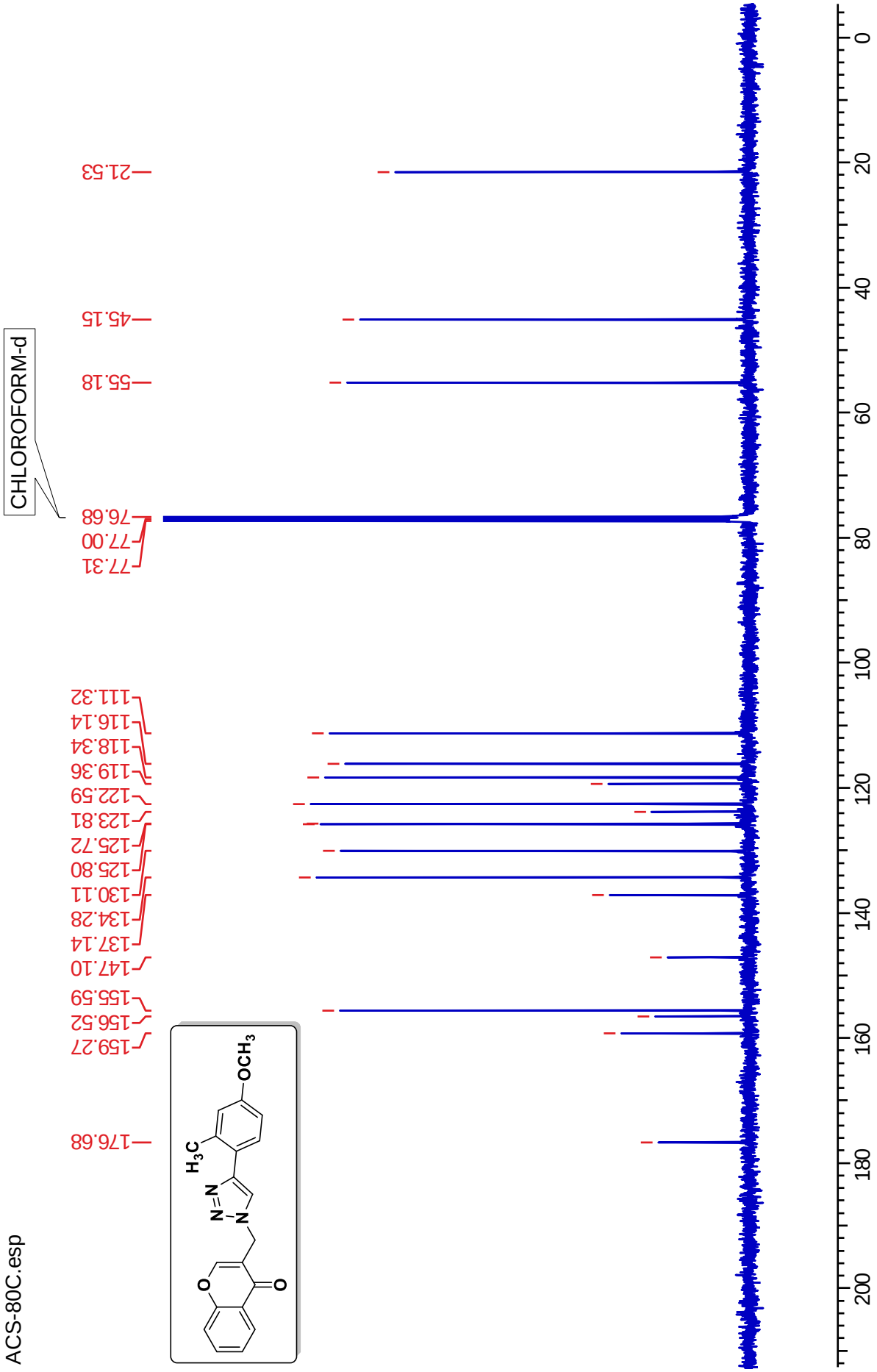

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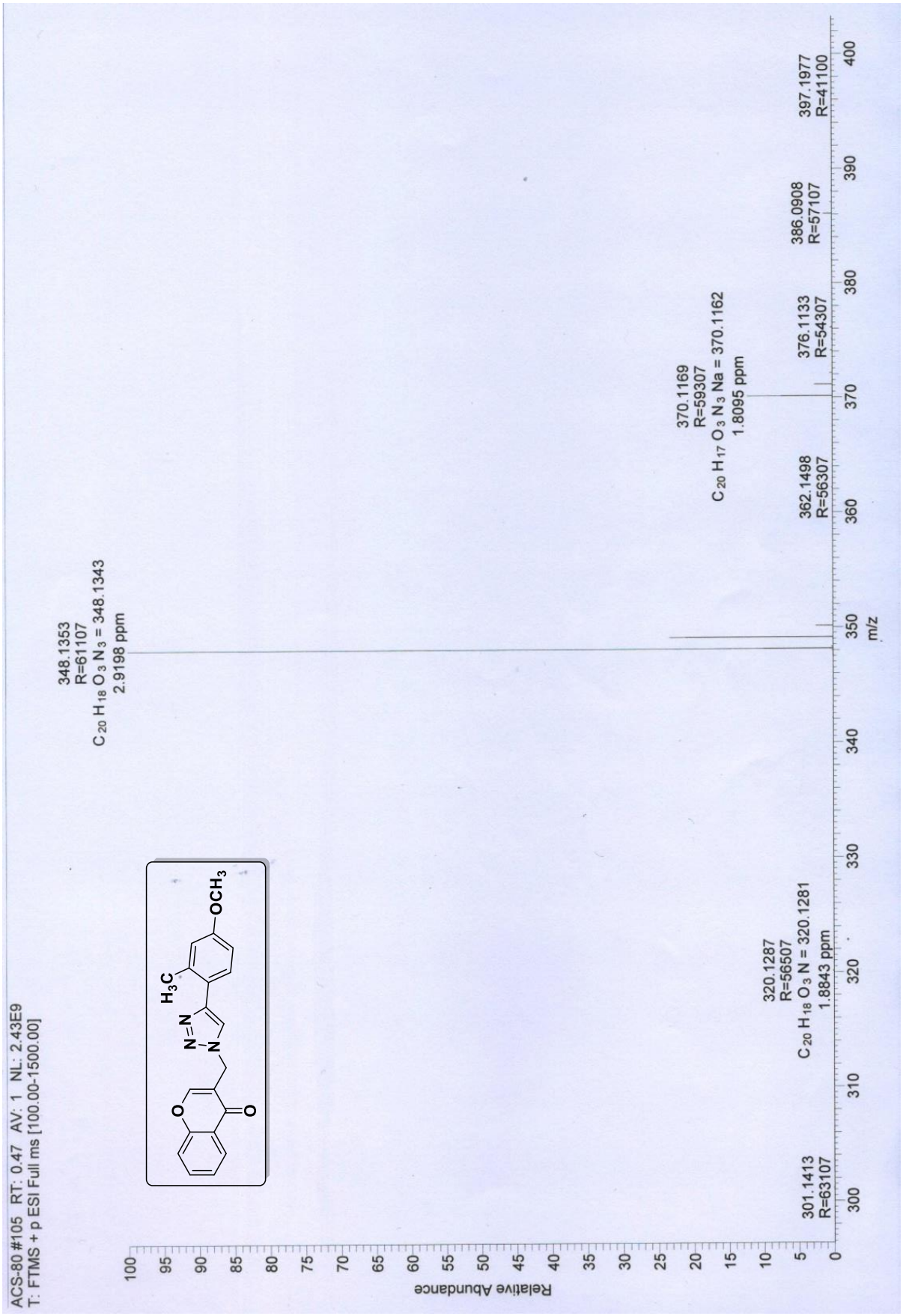
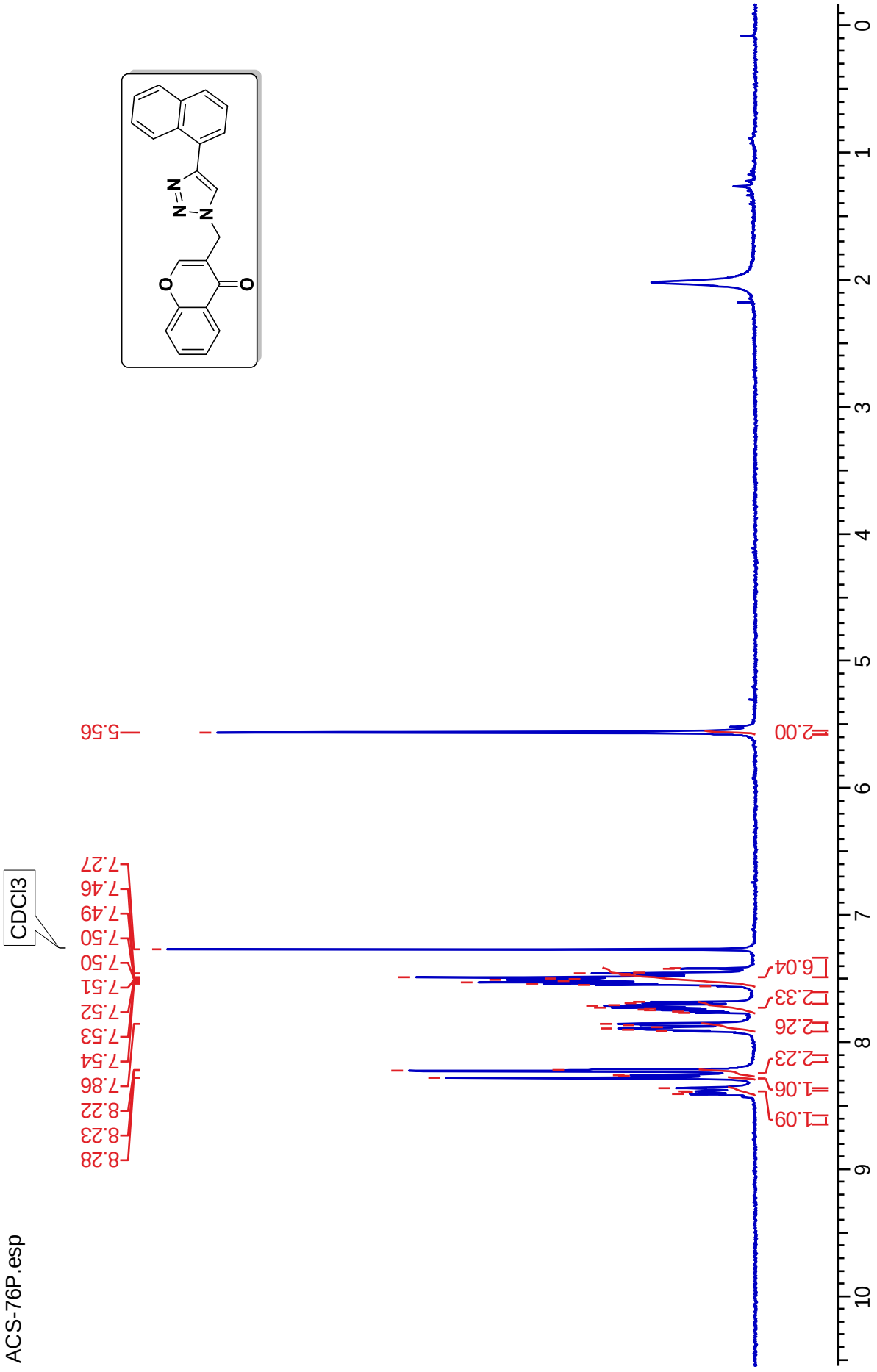
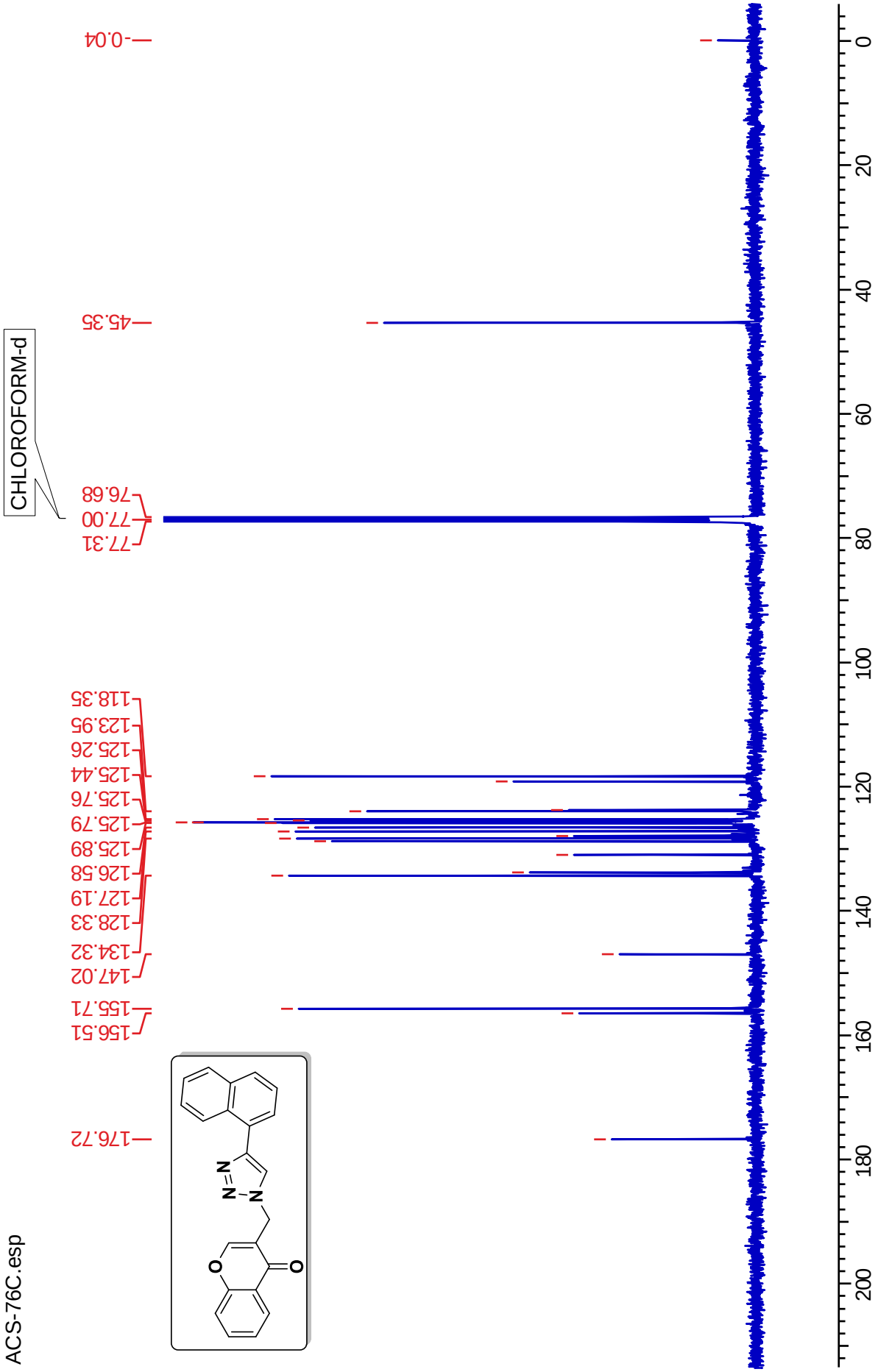


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6k***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6k***:



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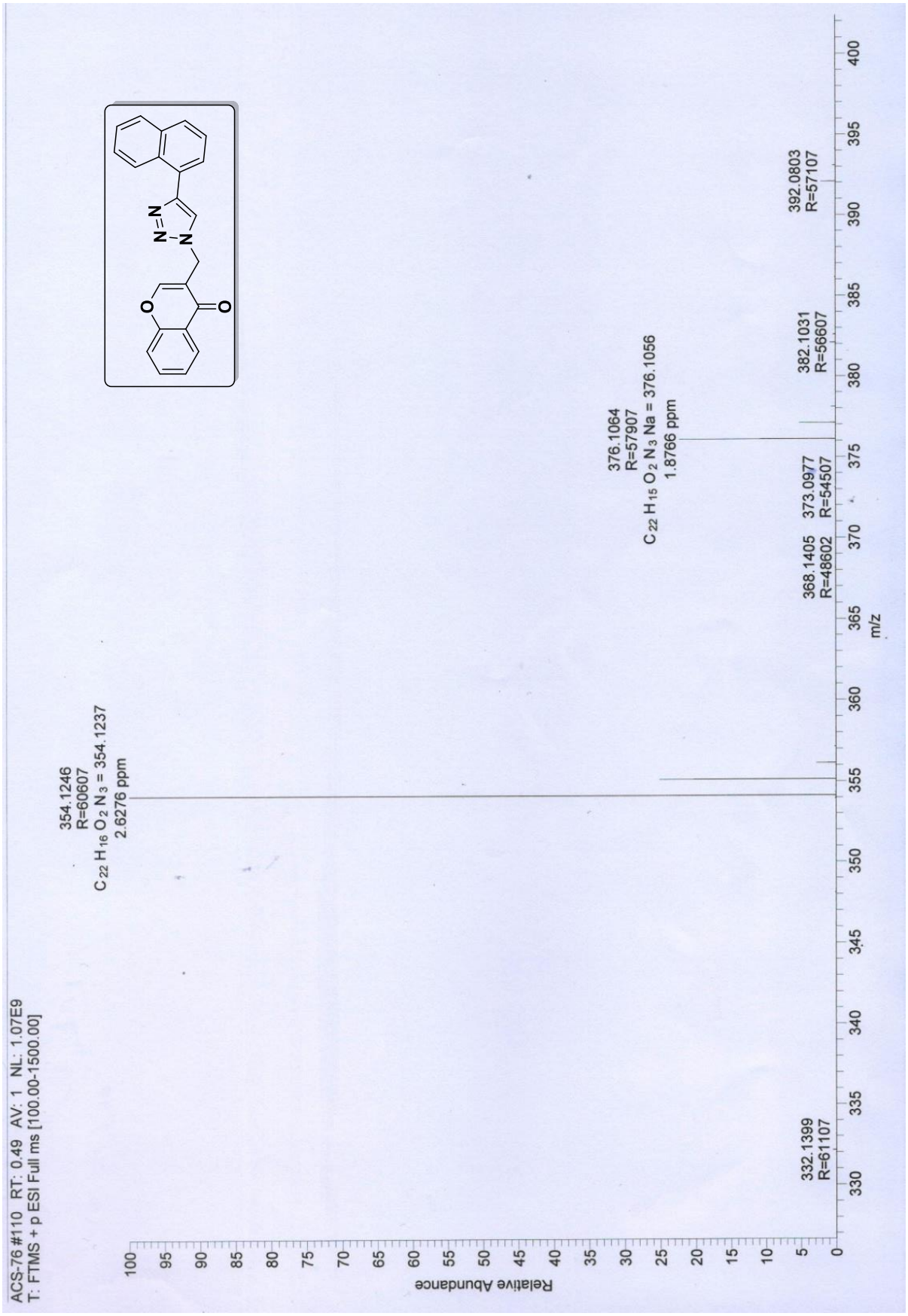
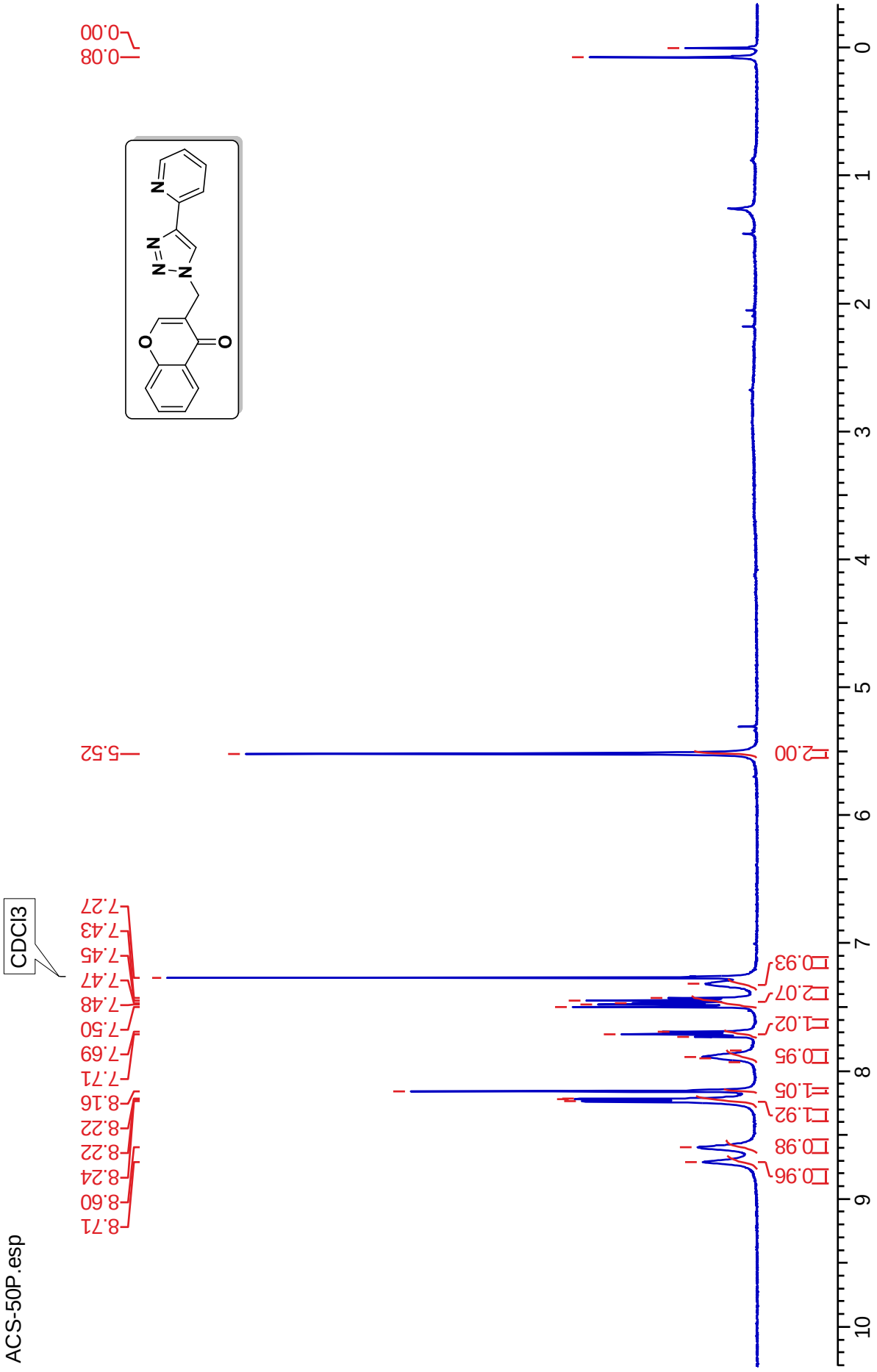
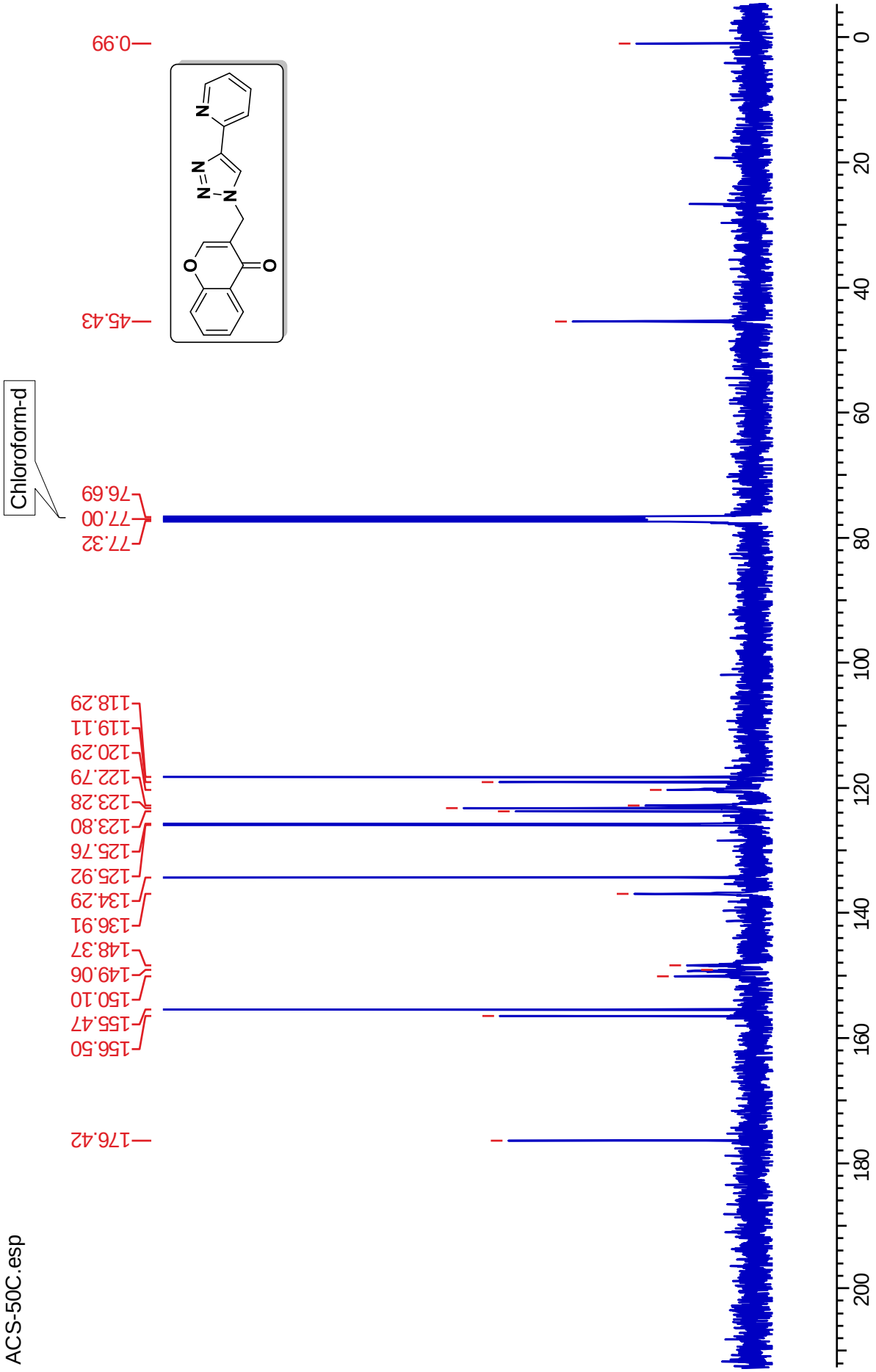


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6l***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6l***:



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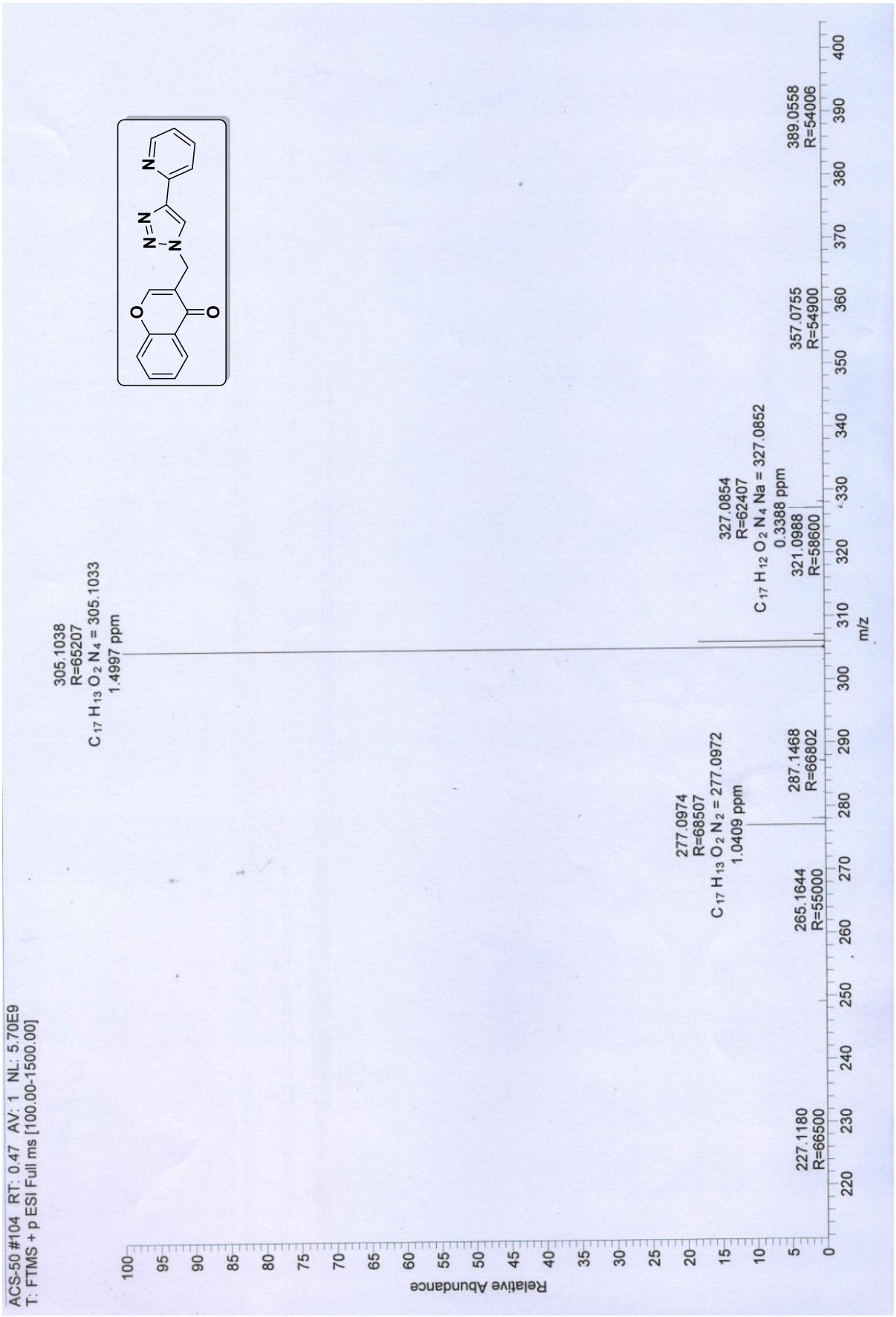
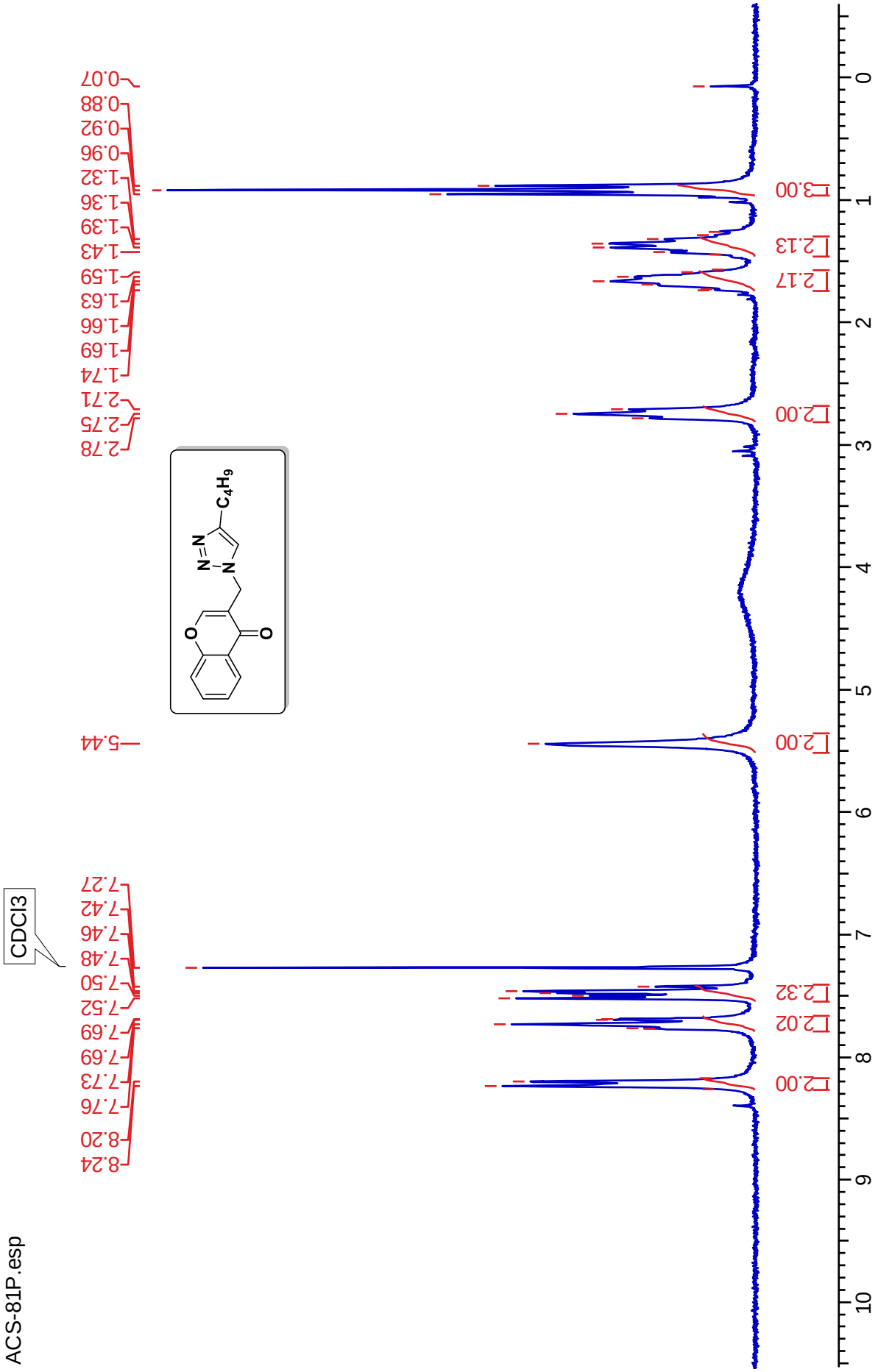
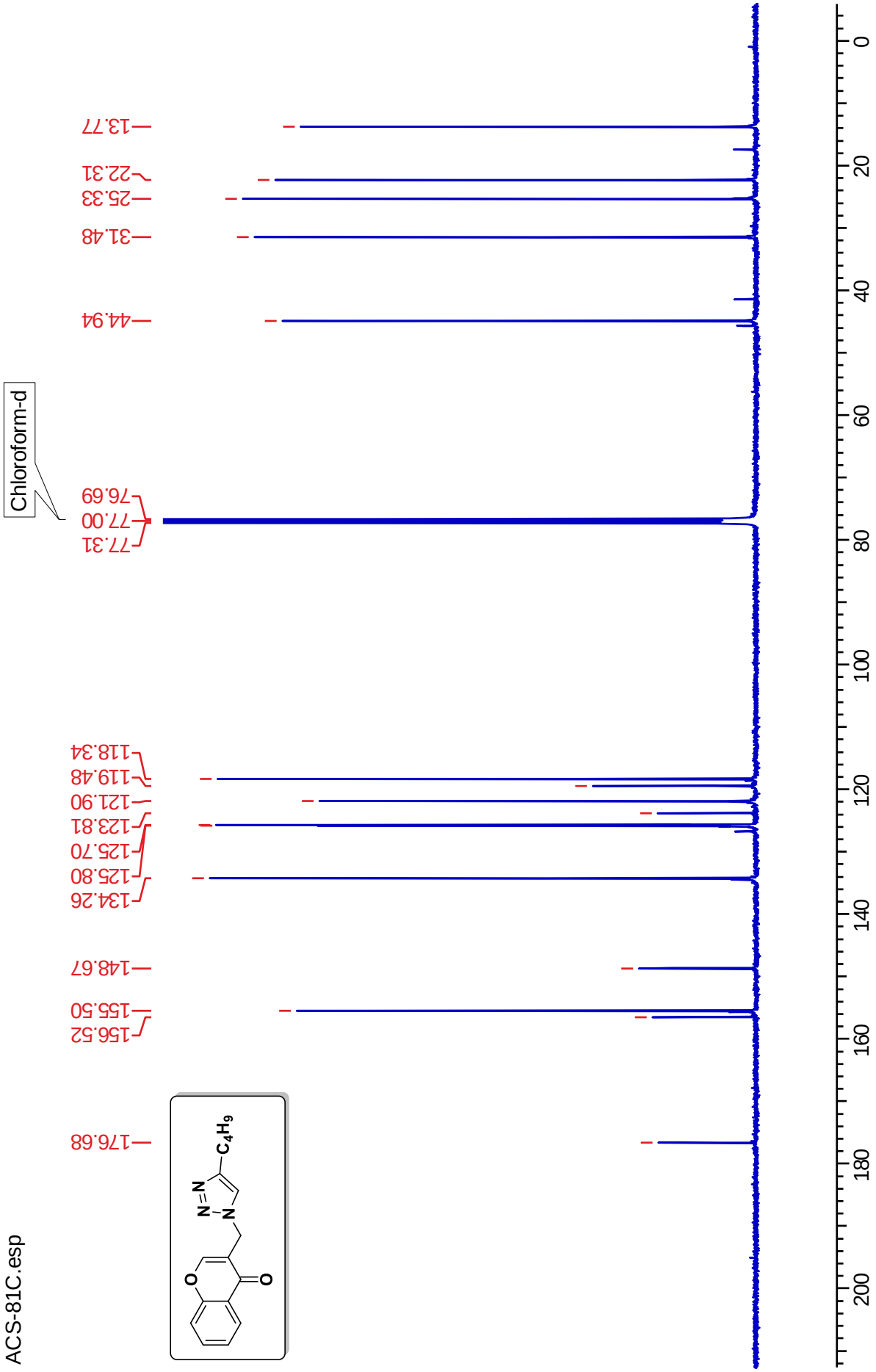


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6m***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6m***:



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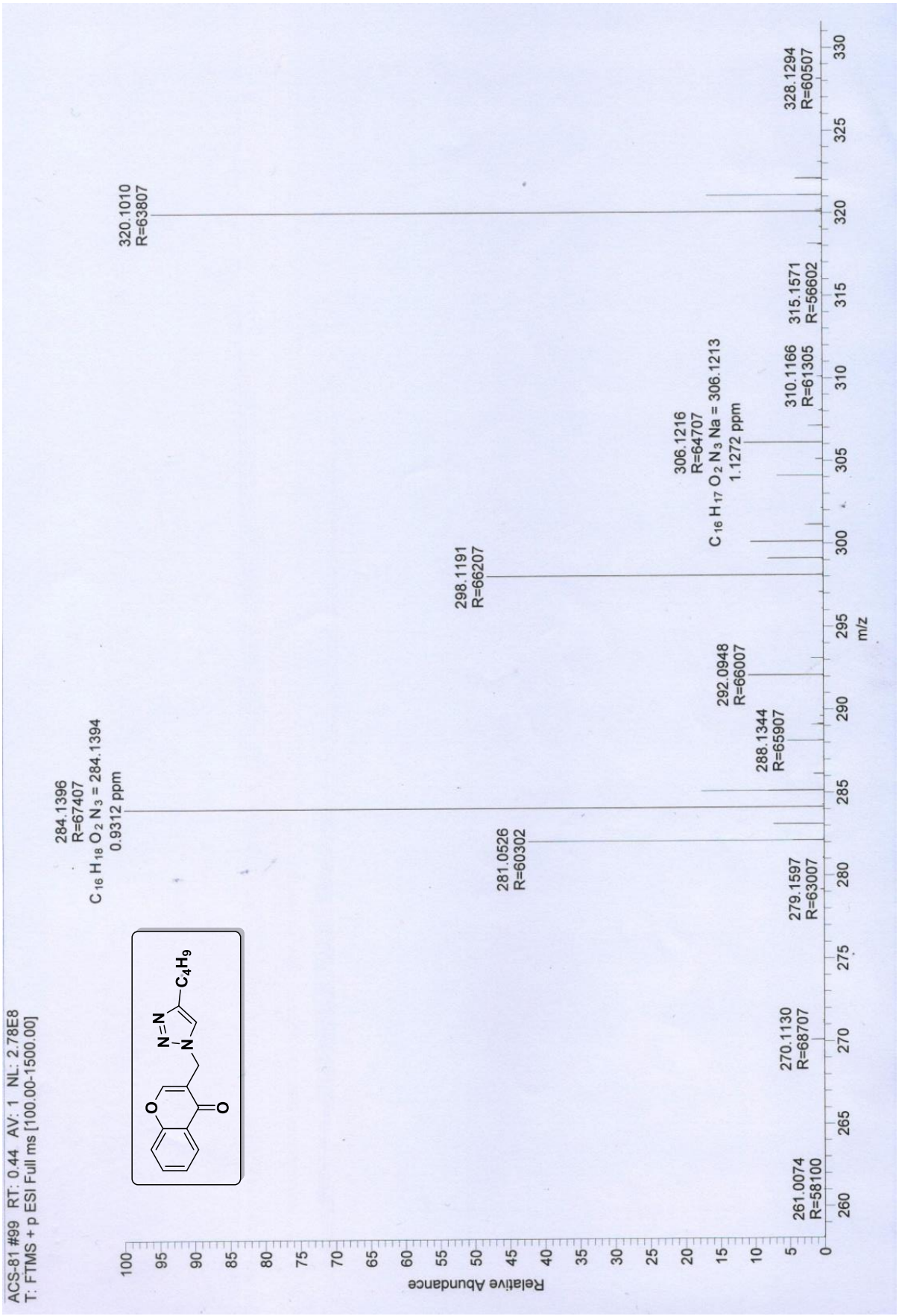
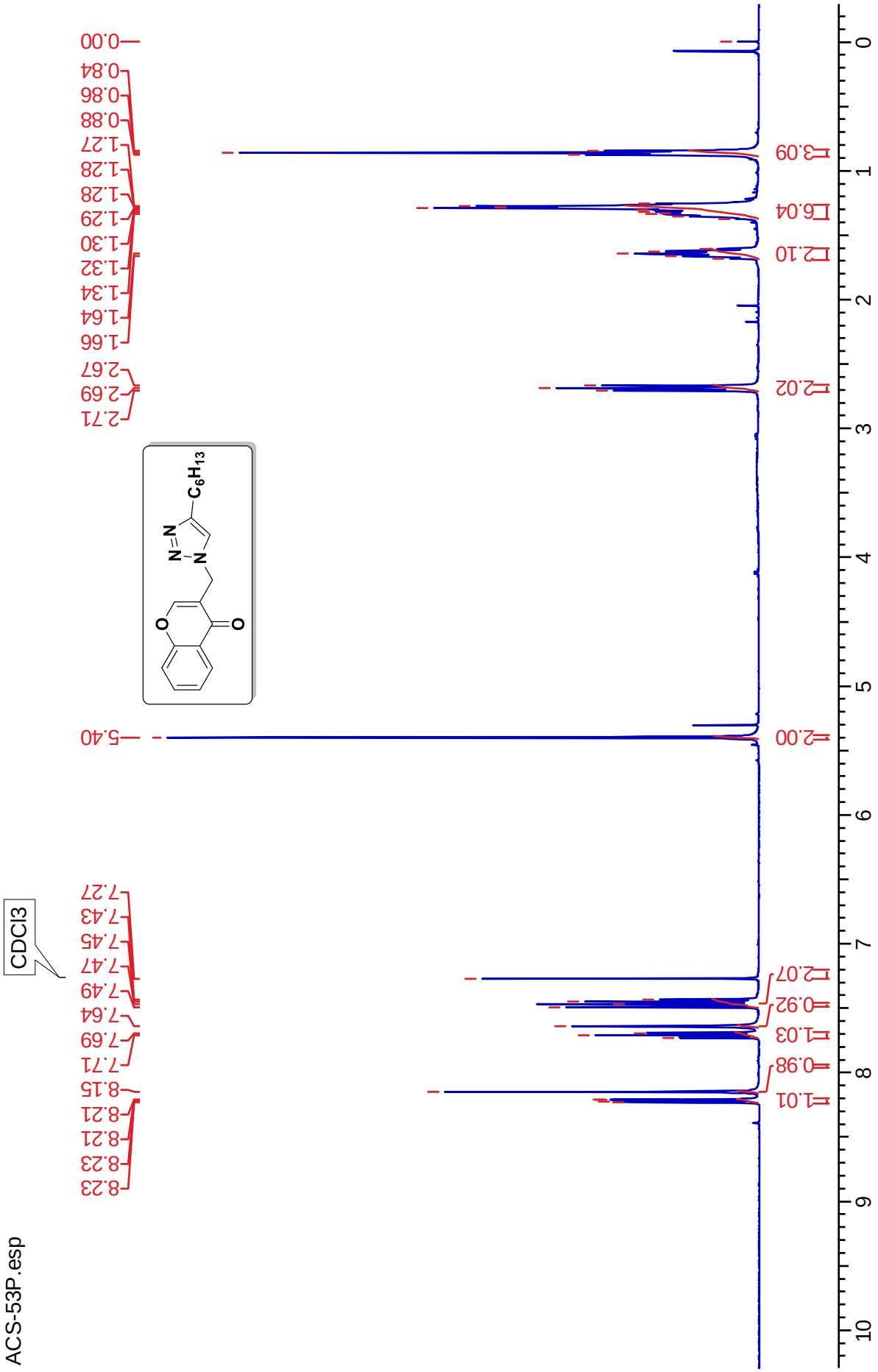
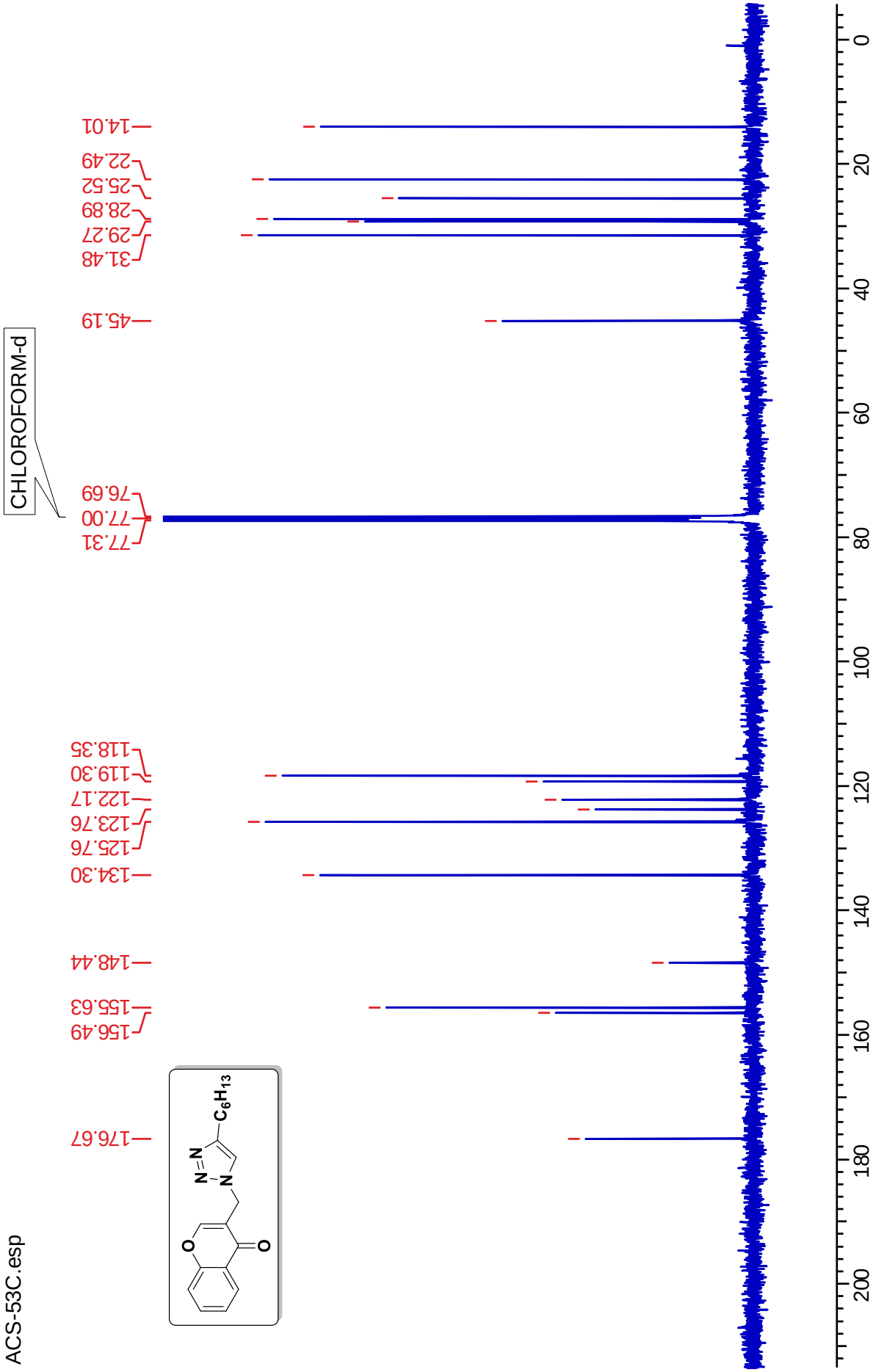


^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6n***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6n***:



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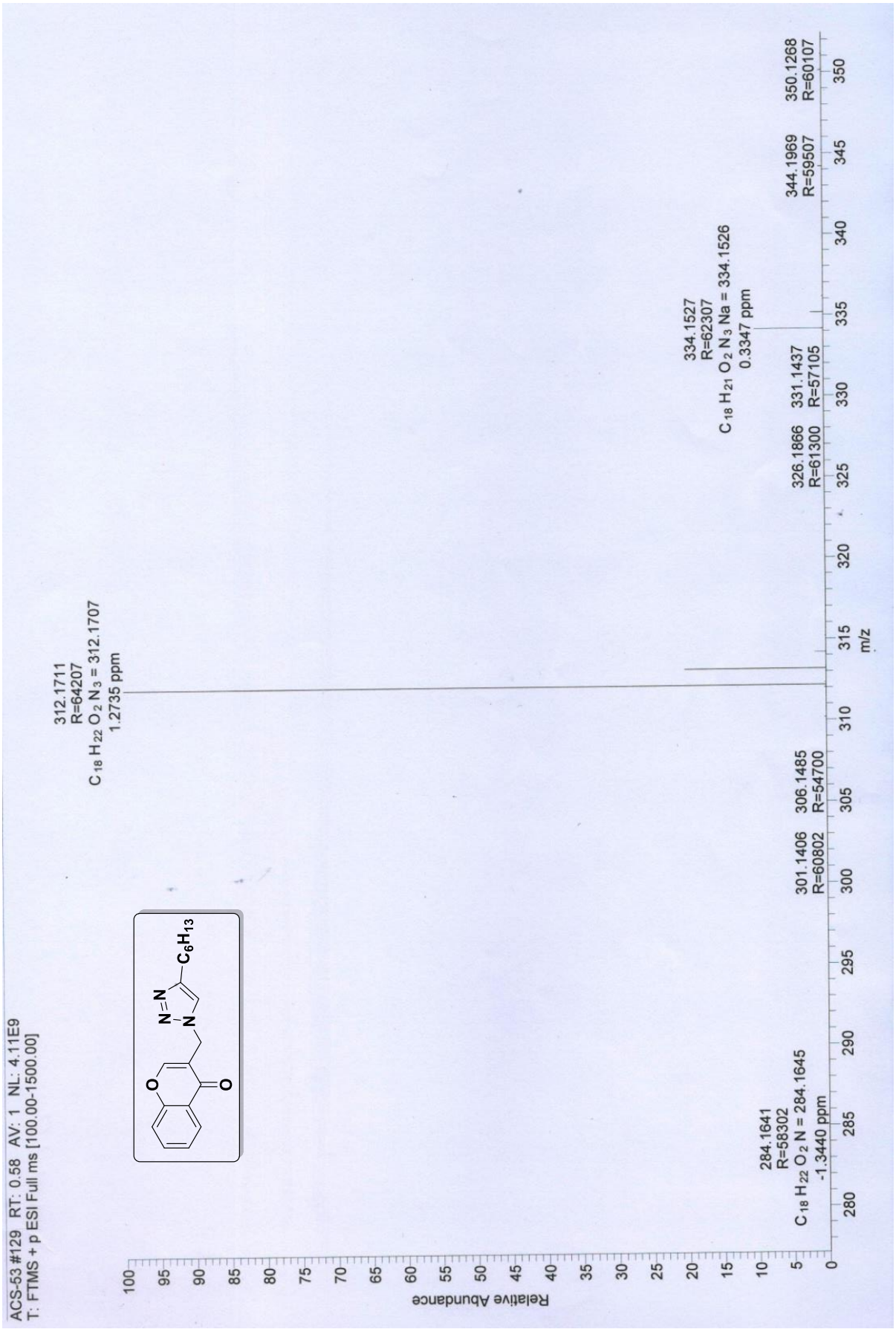
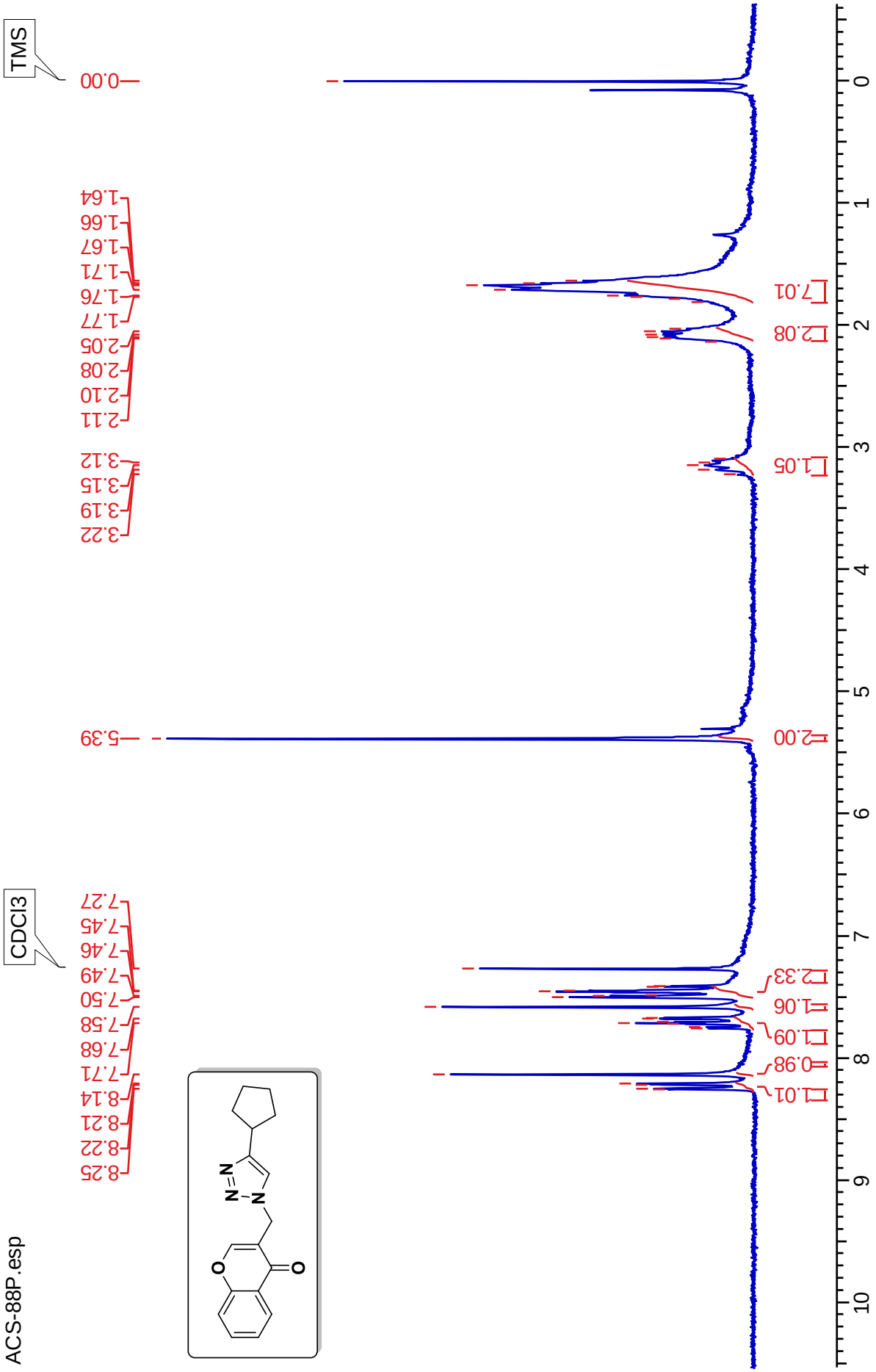
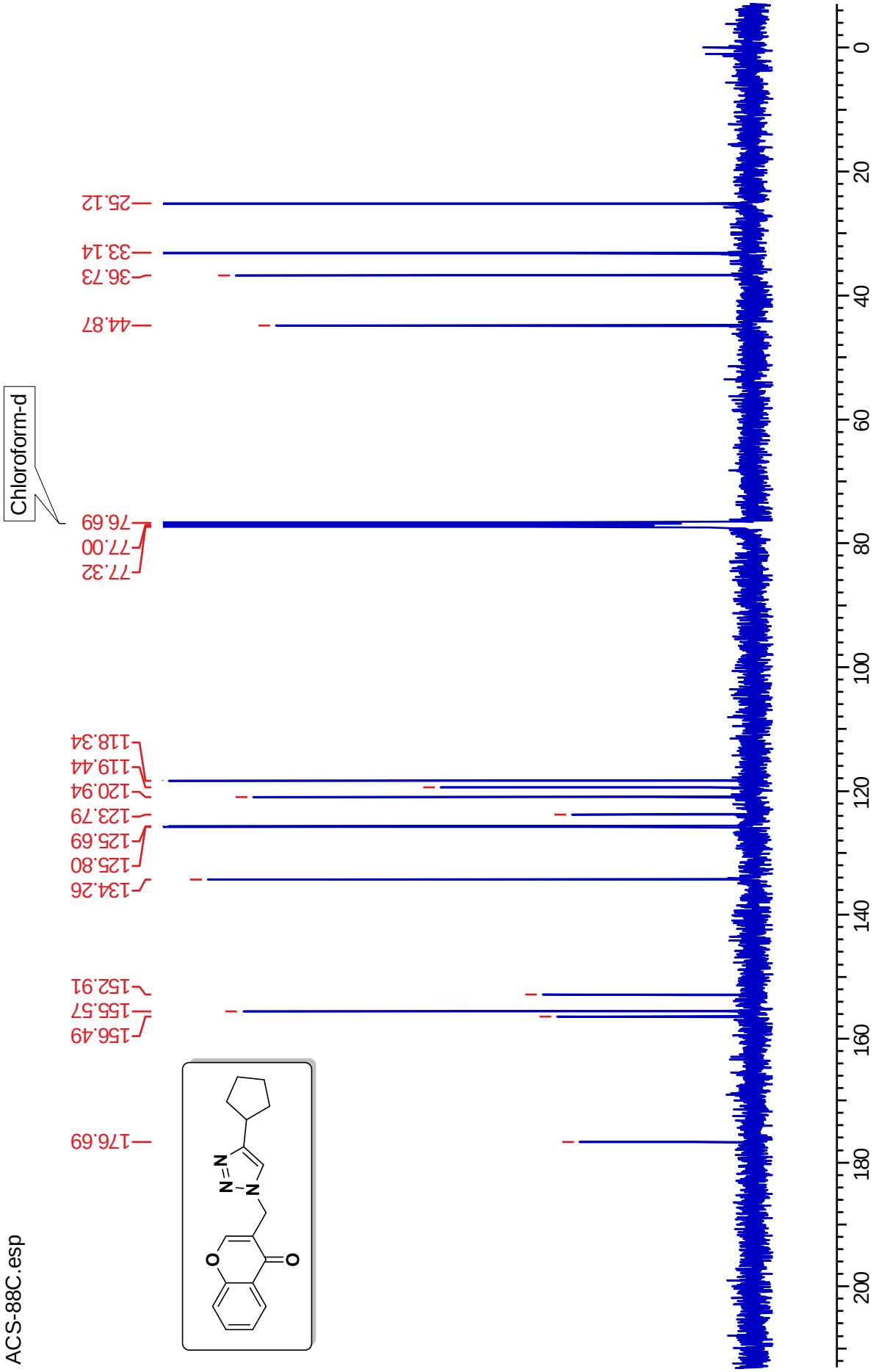


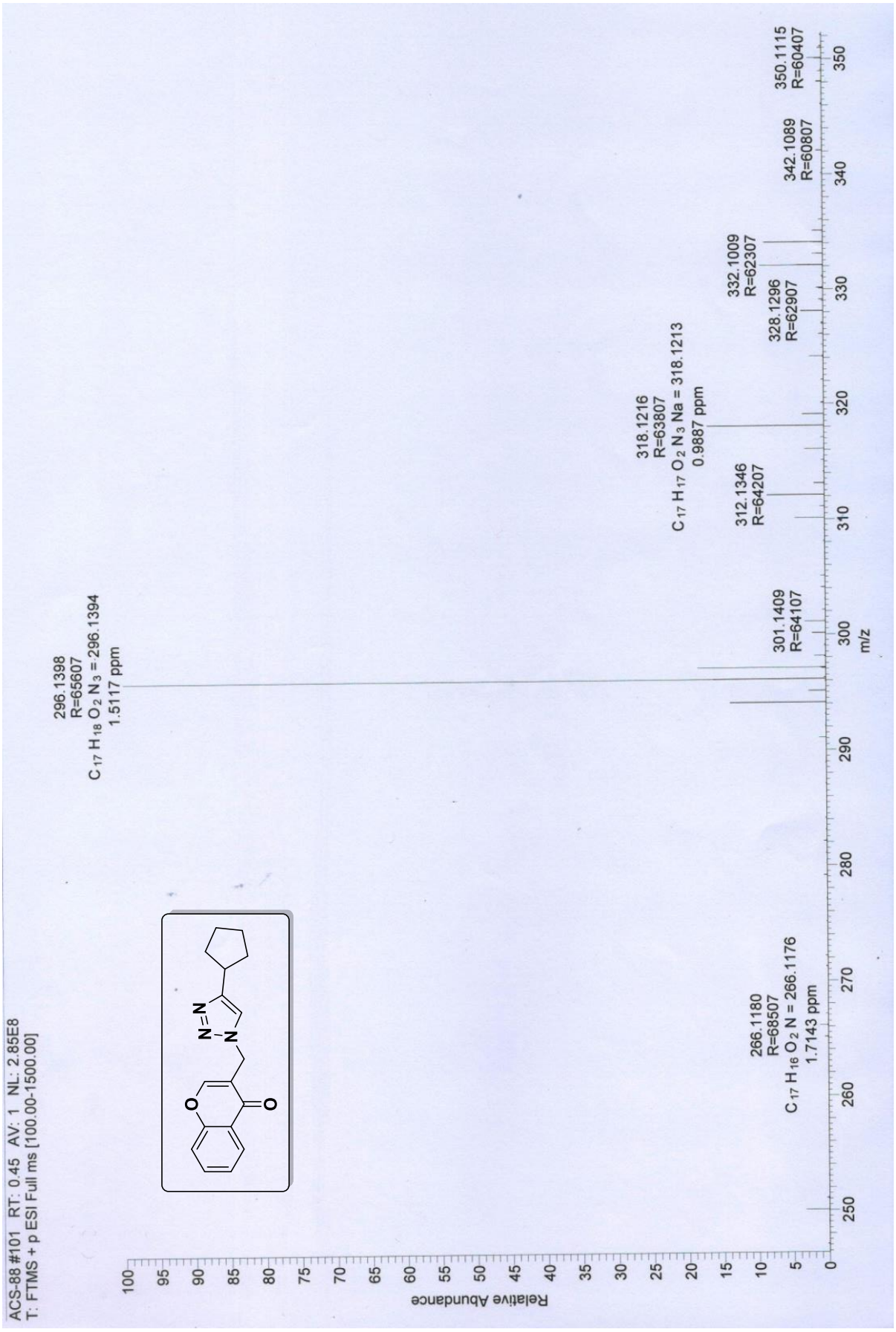
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6o***:



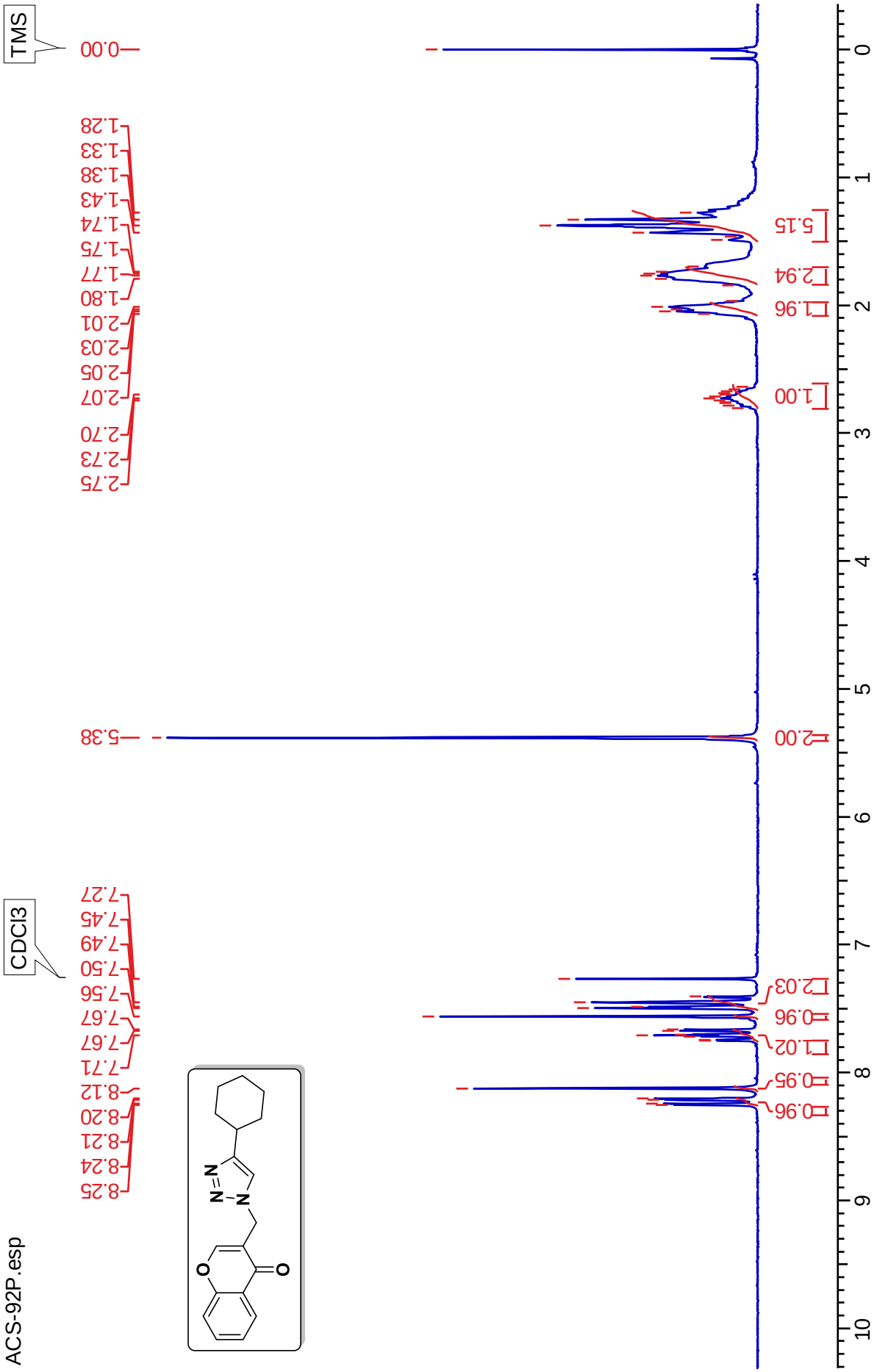
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6o***:



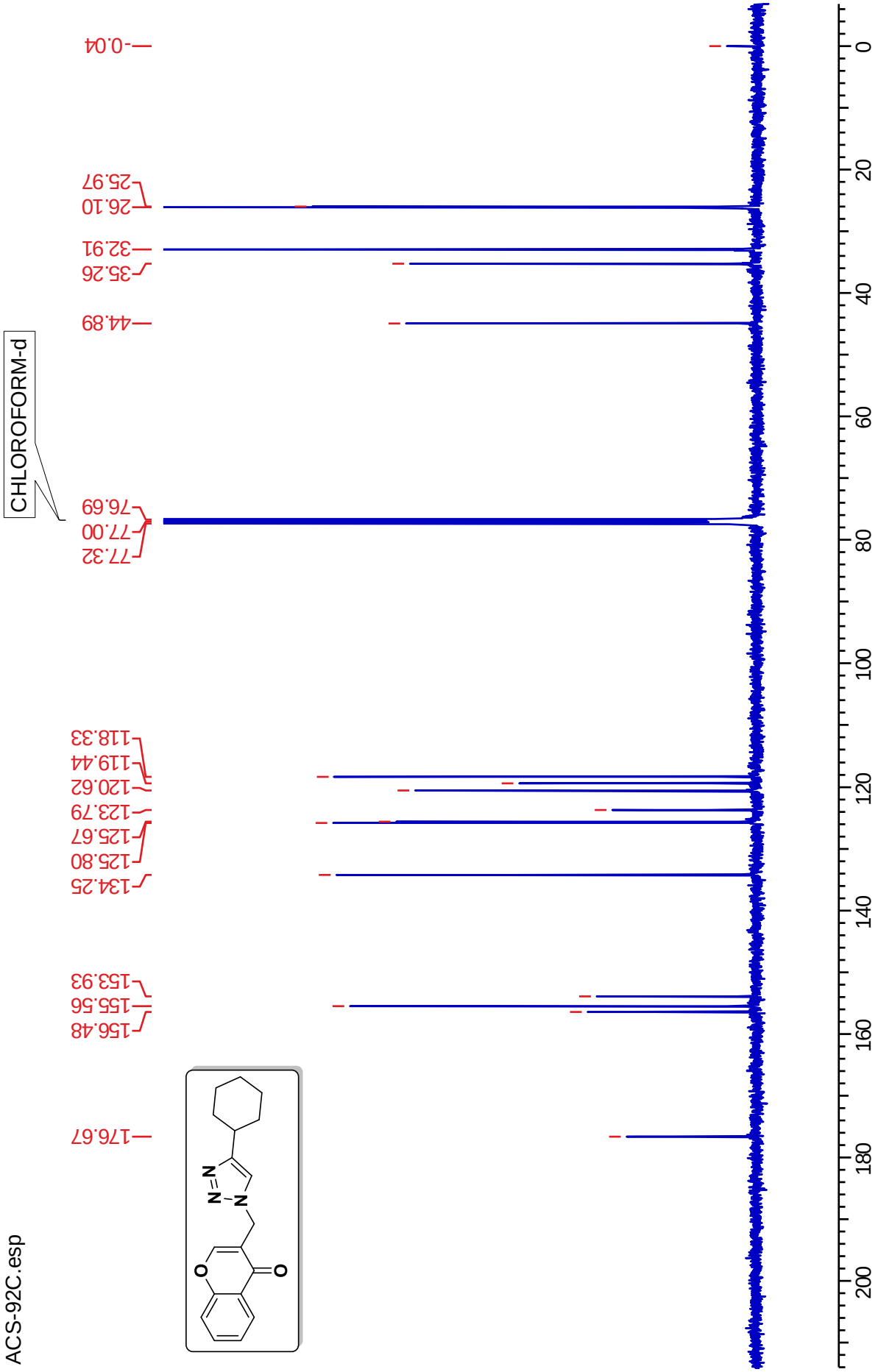
HRMS of compound ***6o***:



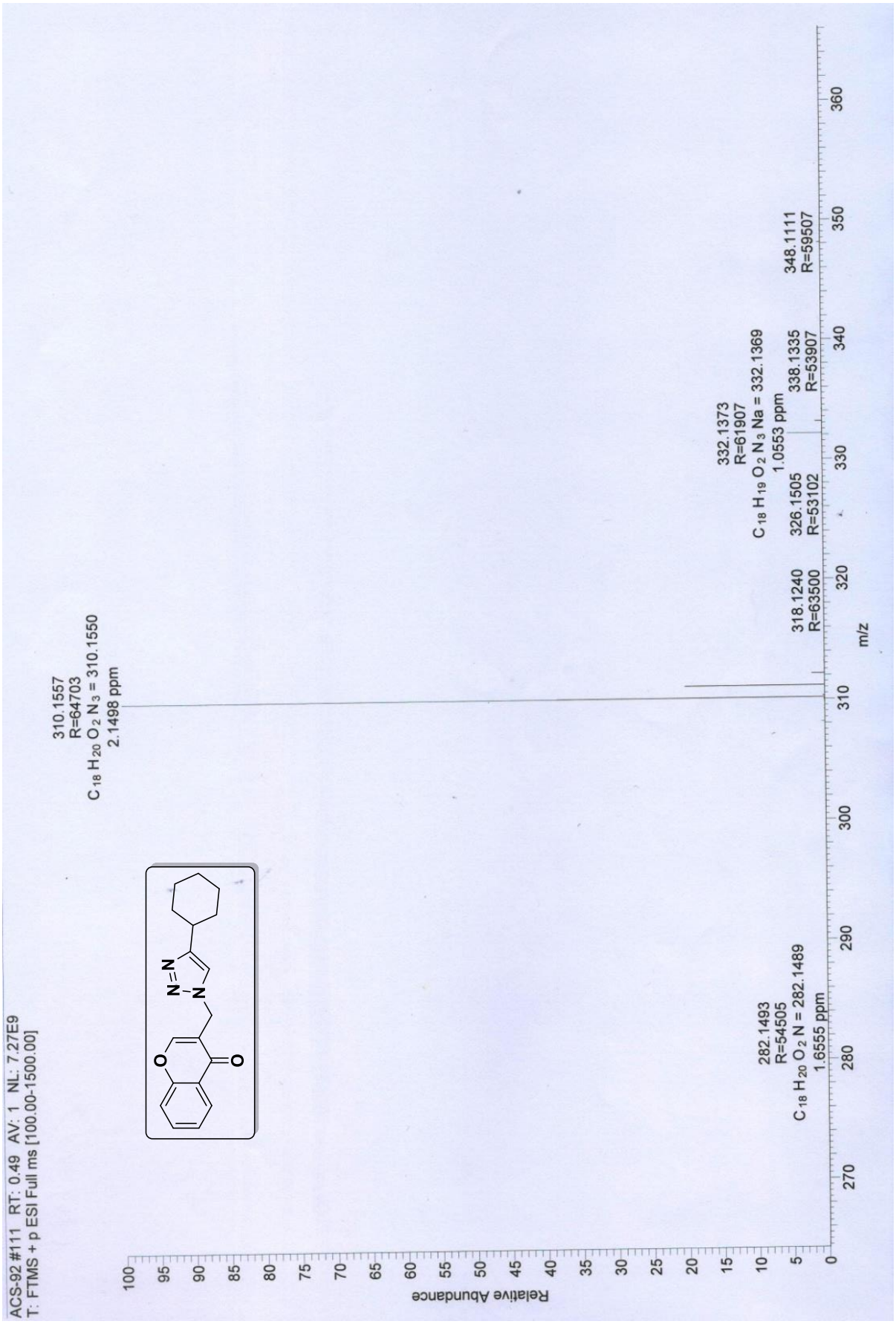
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6p***:



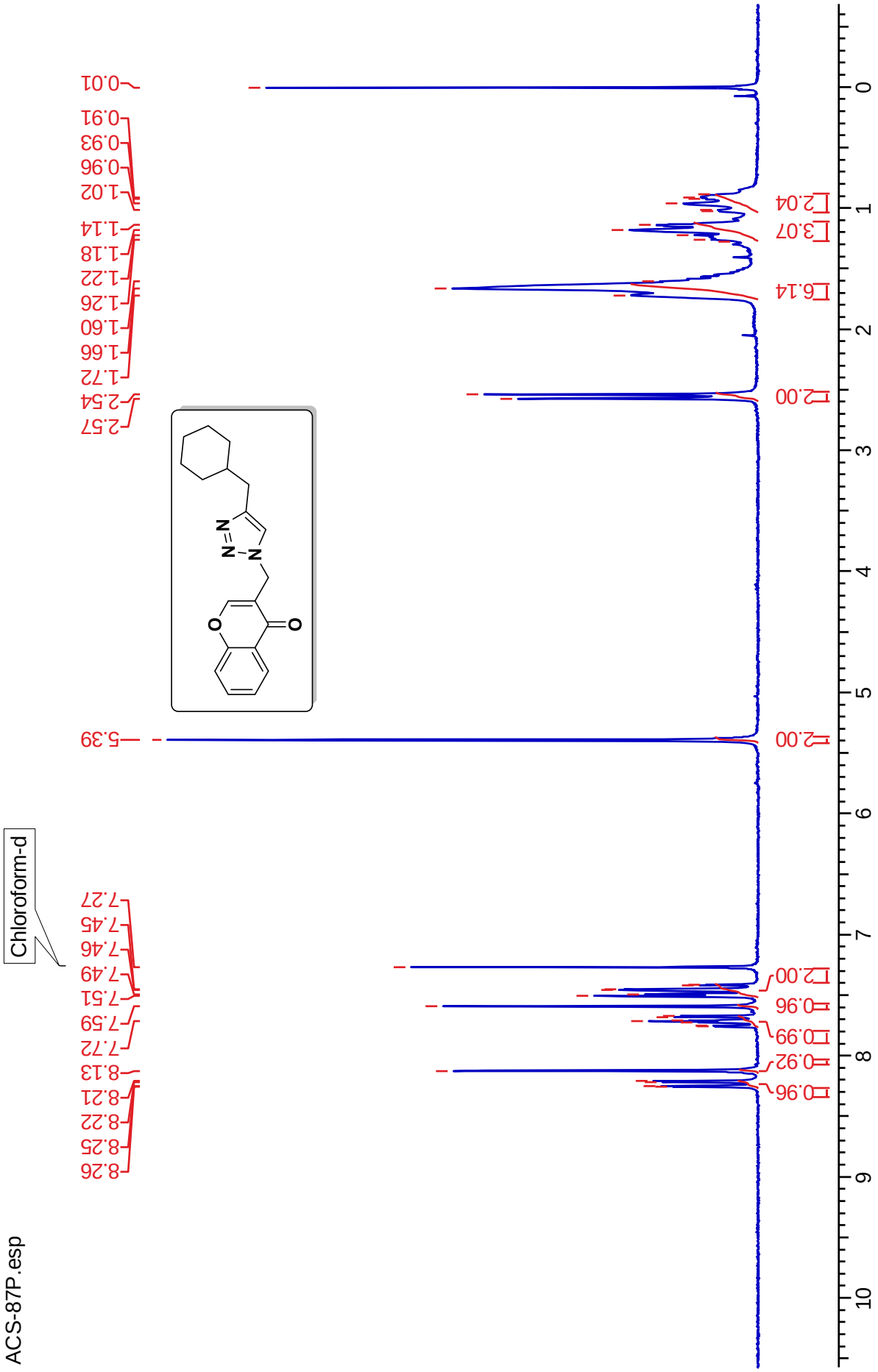
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6p***:



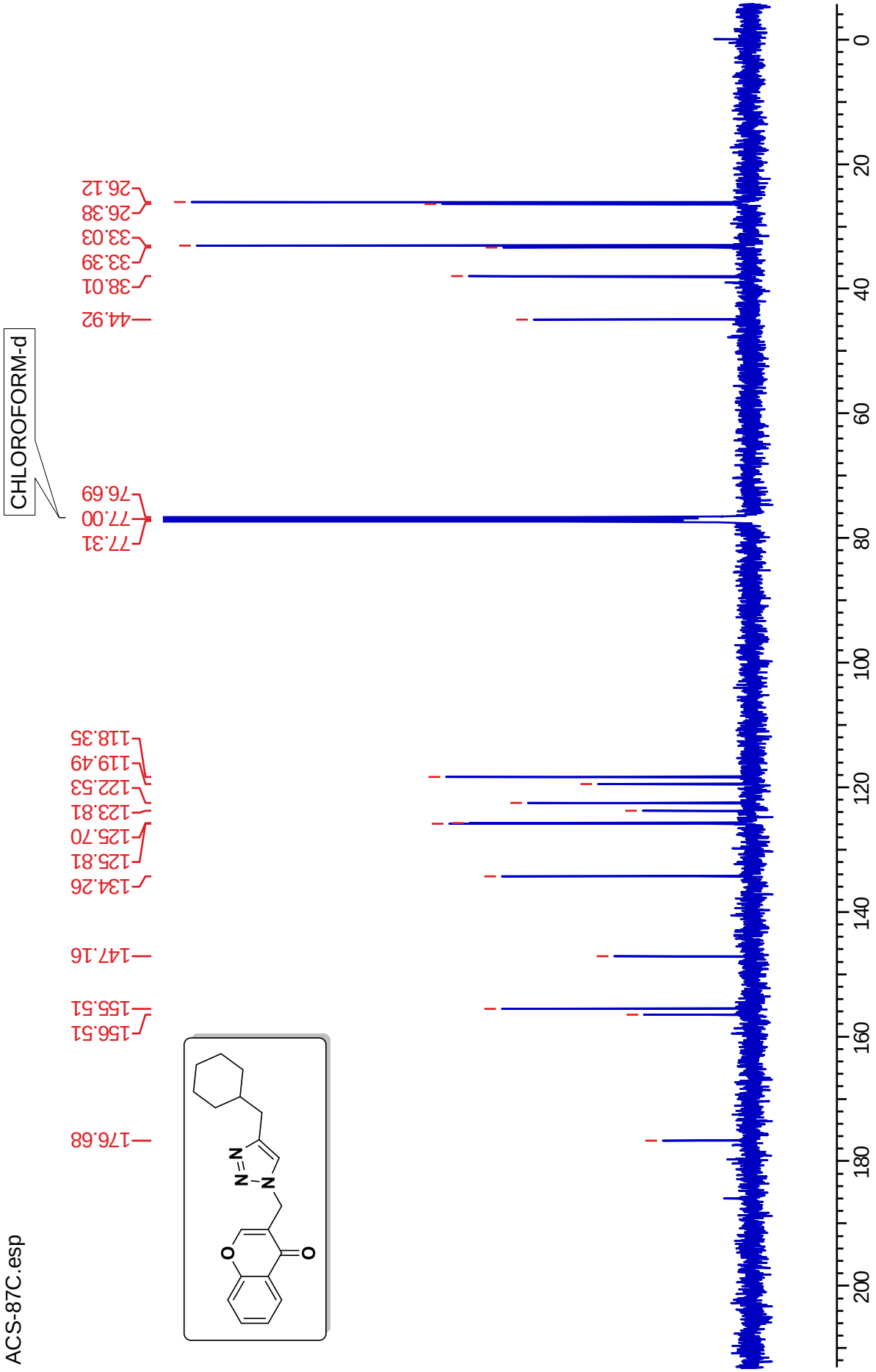
HRMS of compound ***6p***:



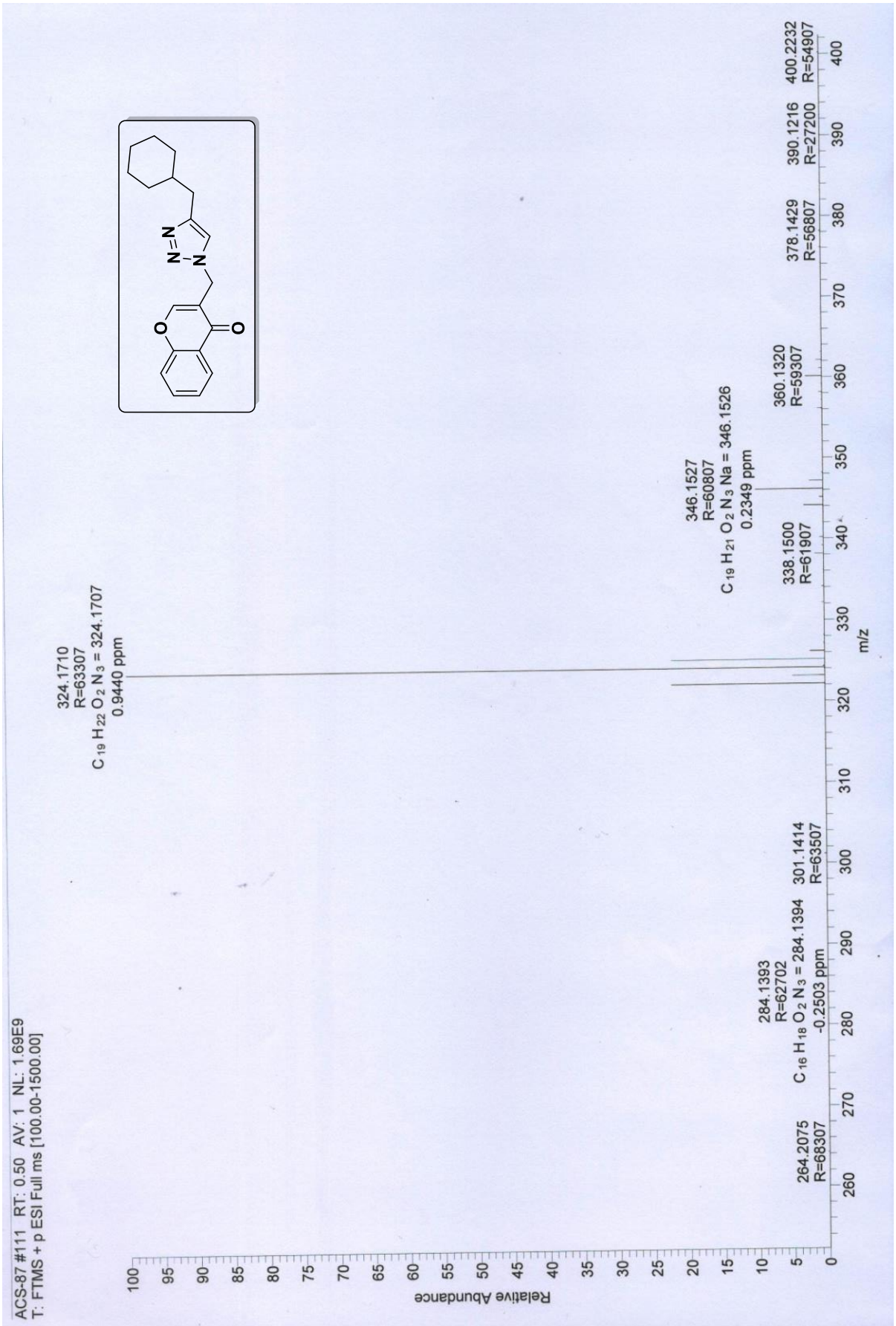
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6q***:



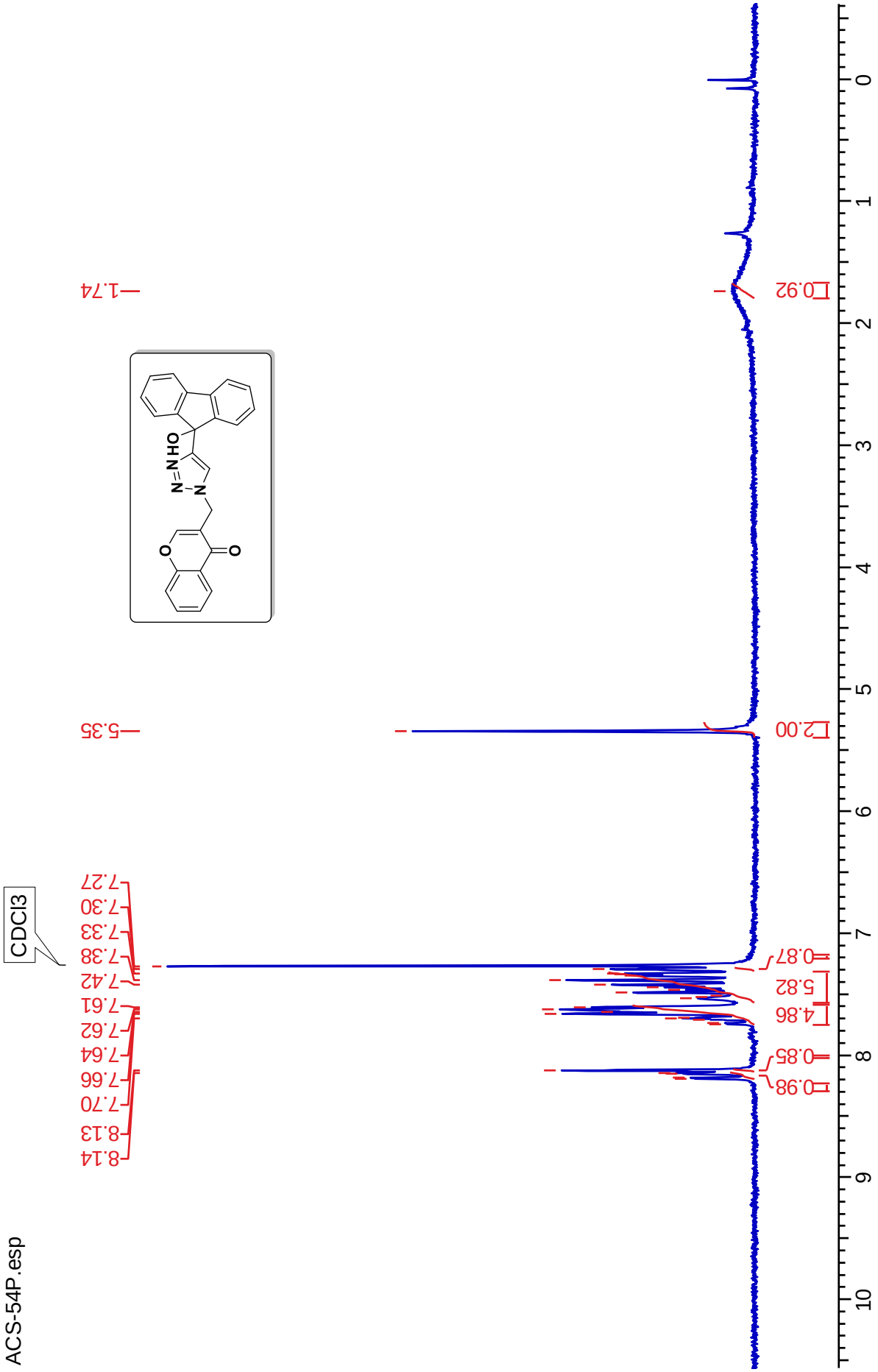
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6q***:



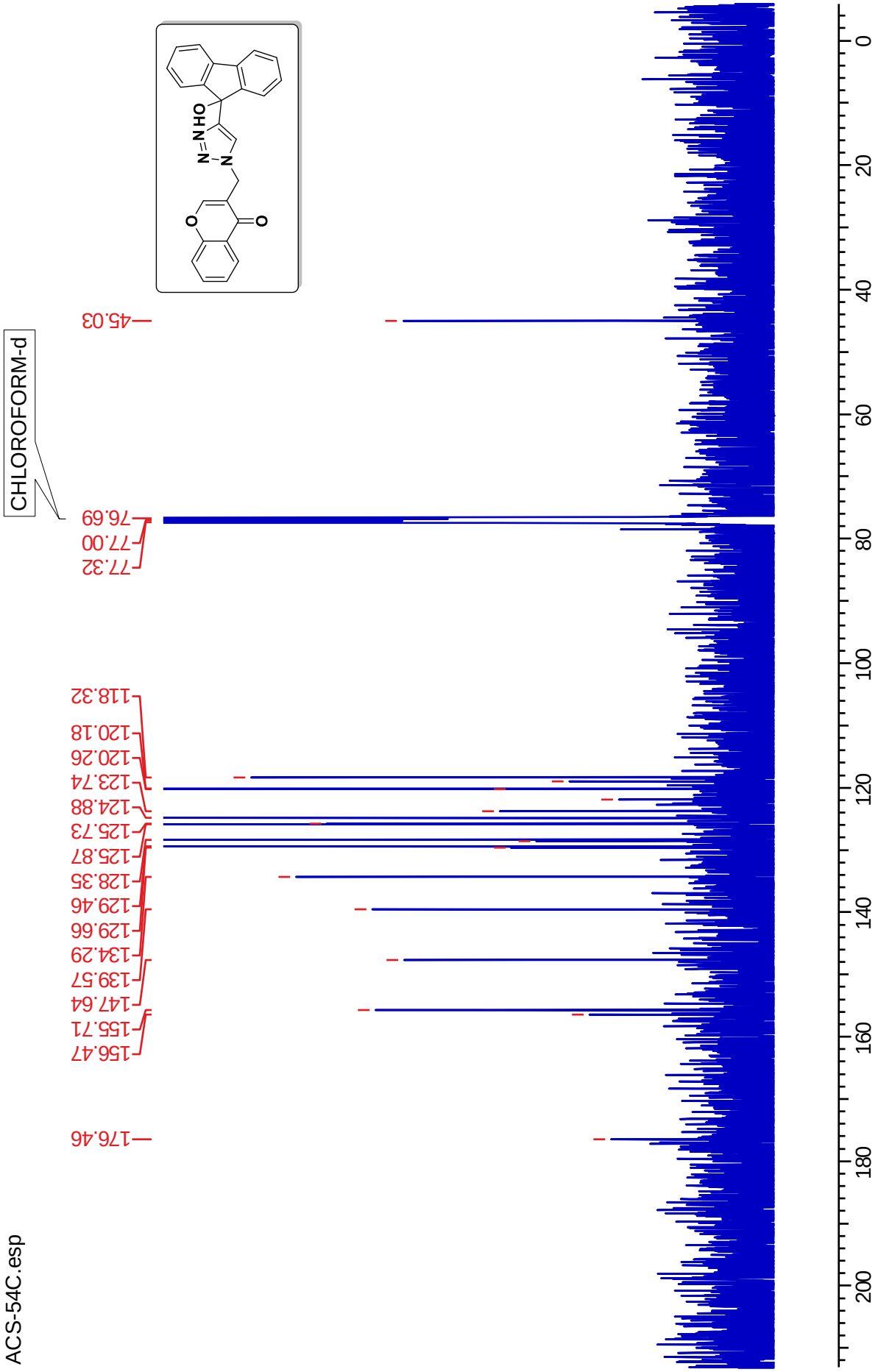
HRMS of compound ***6q***:



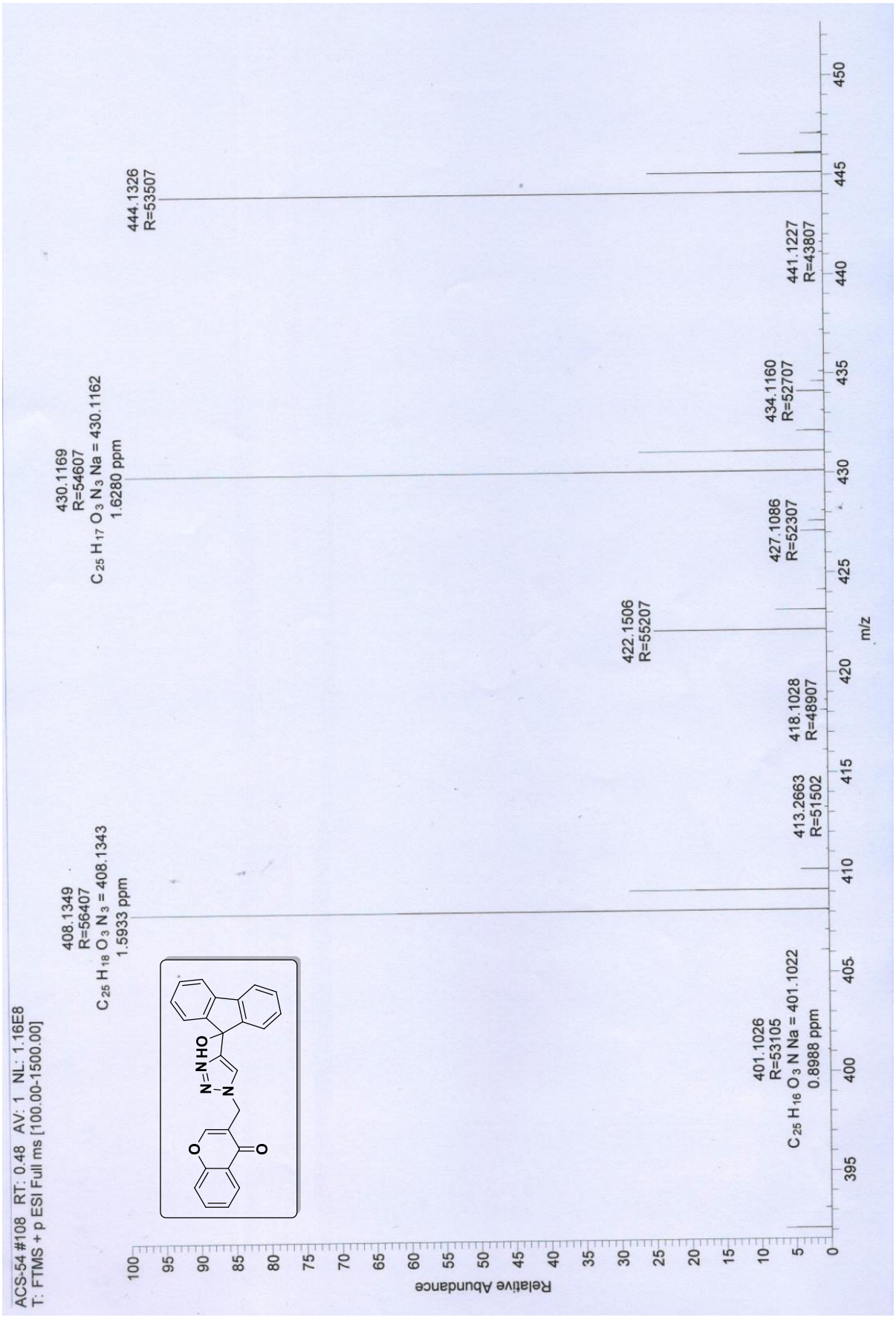
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6r***:



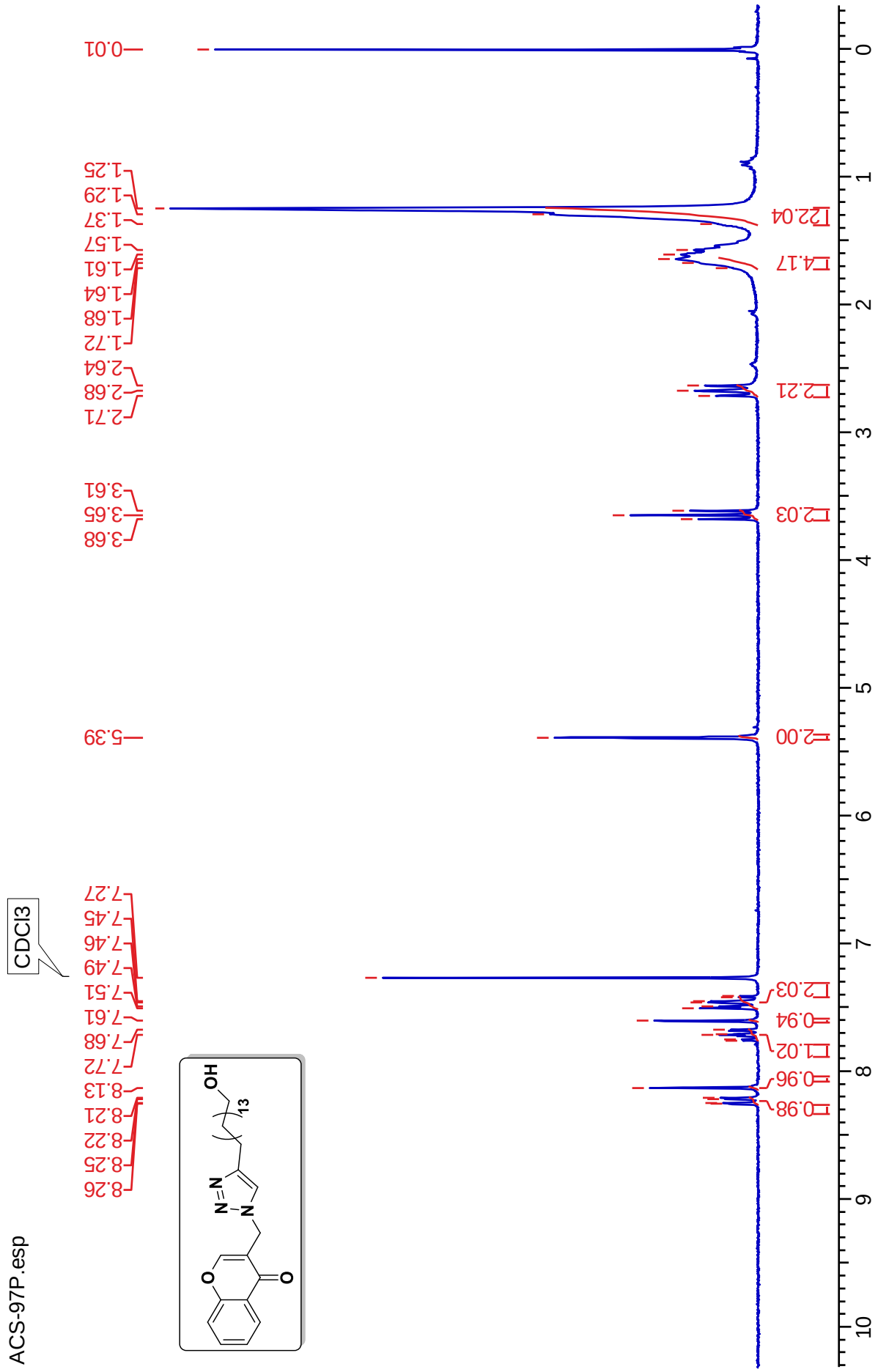
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6r***:



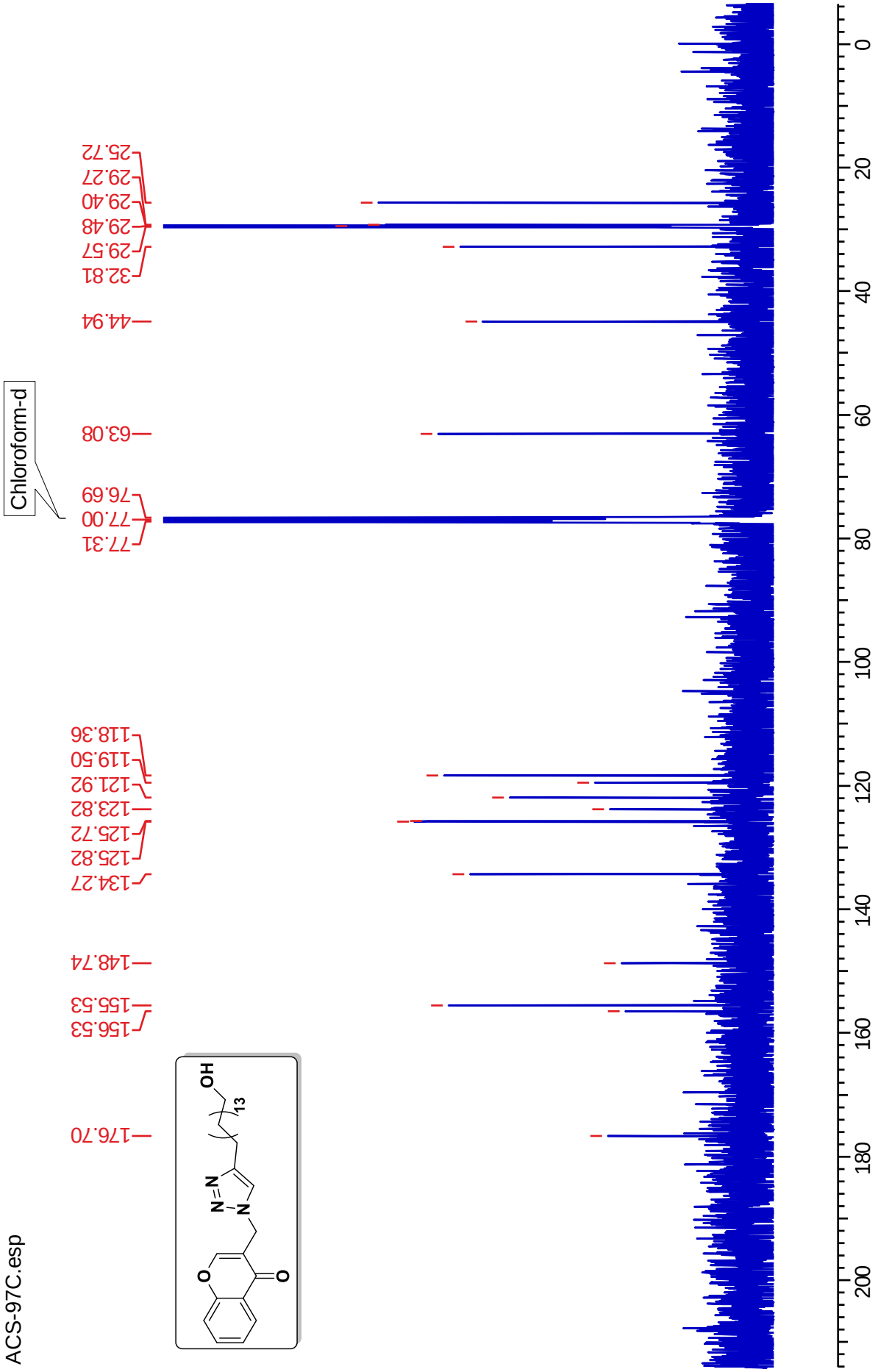
HRMS of compound ***6r***:



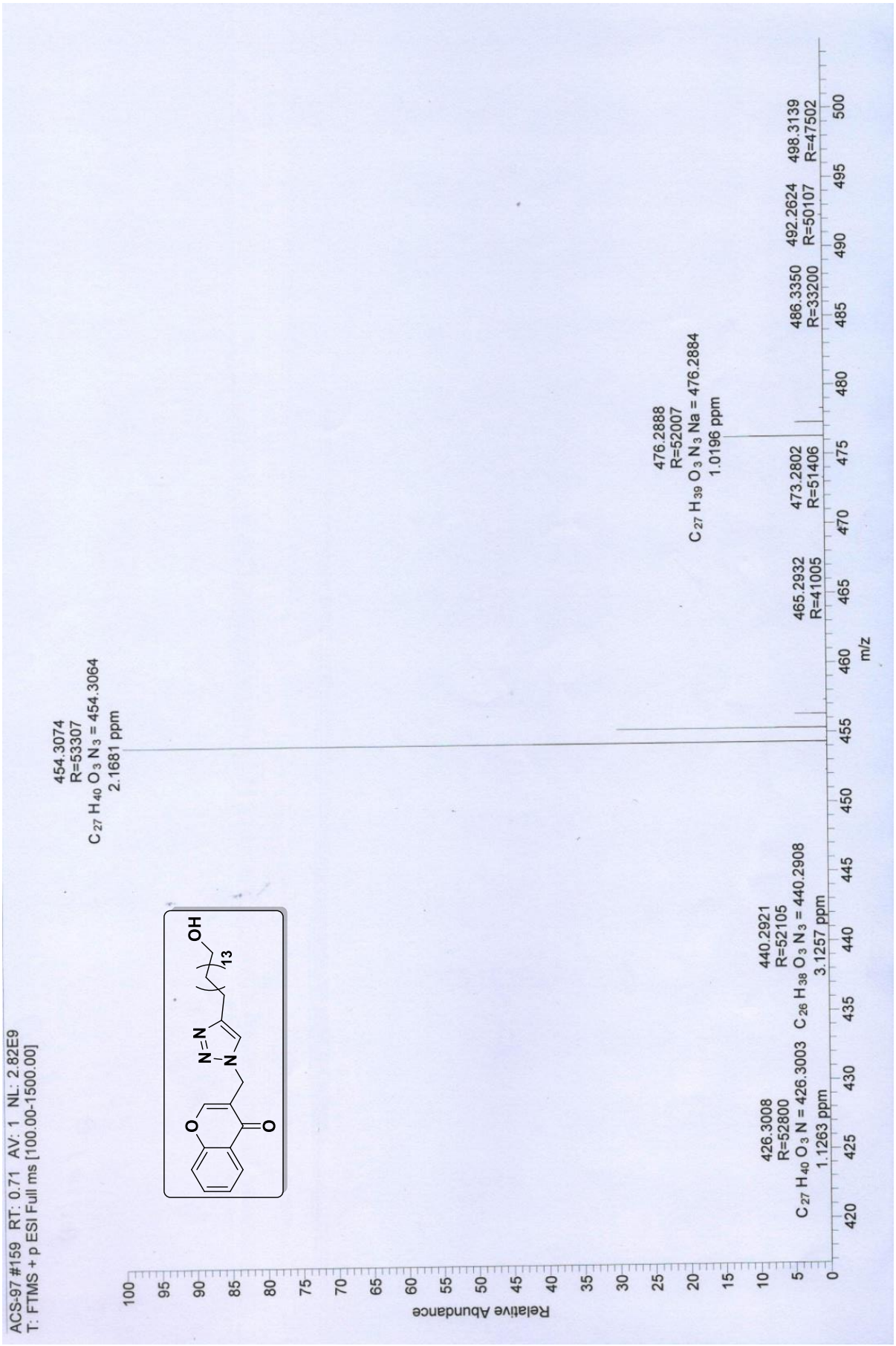
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6s***:



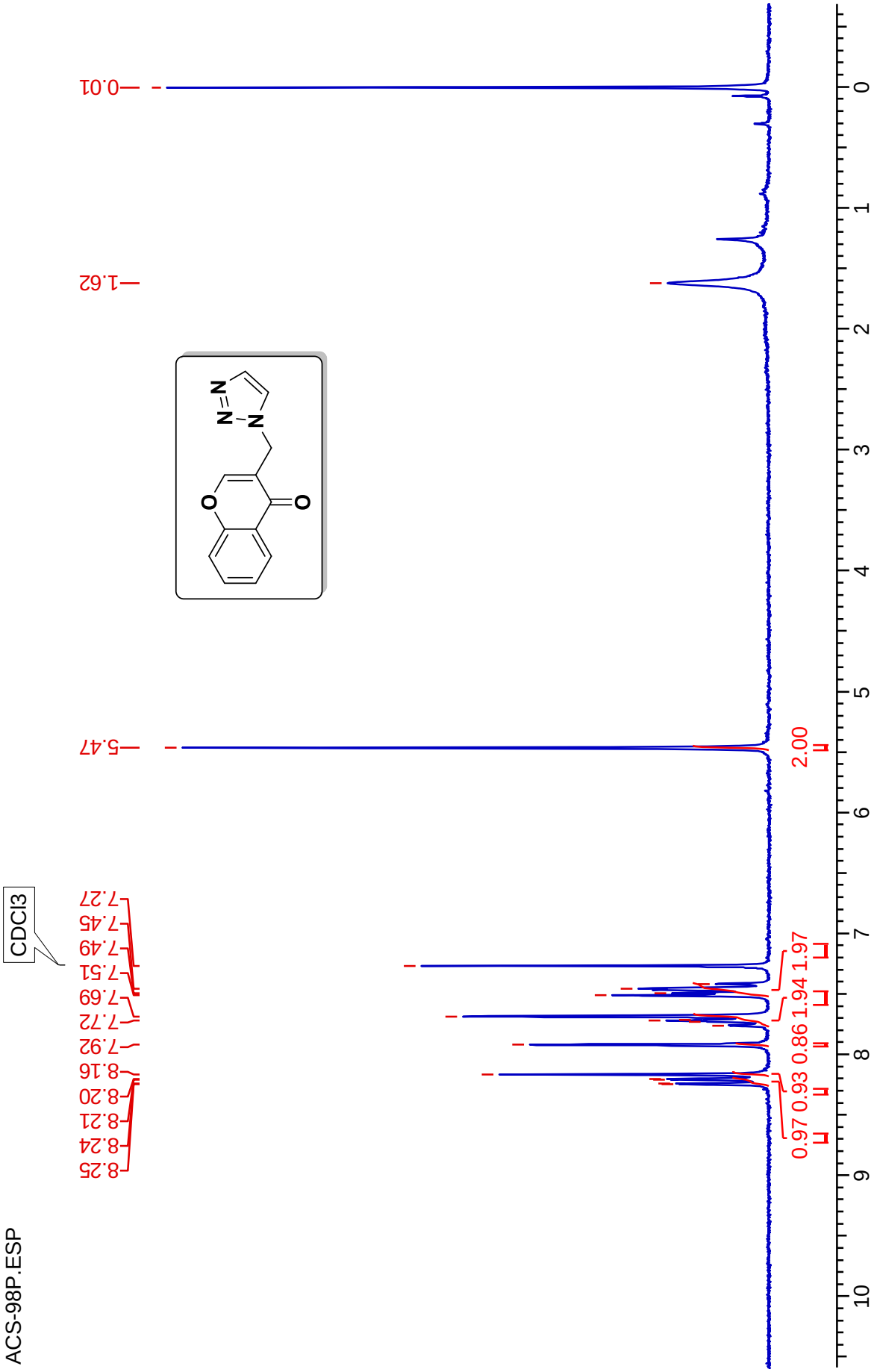
^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6s***:



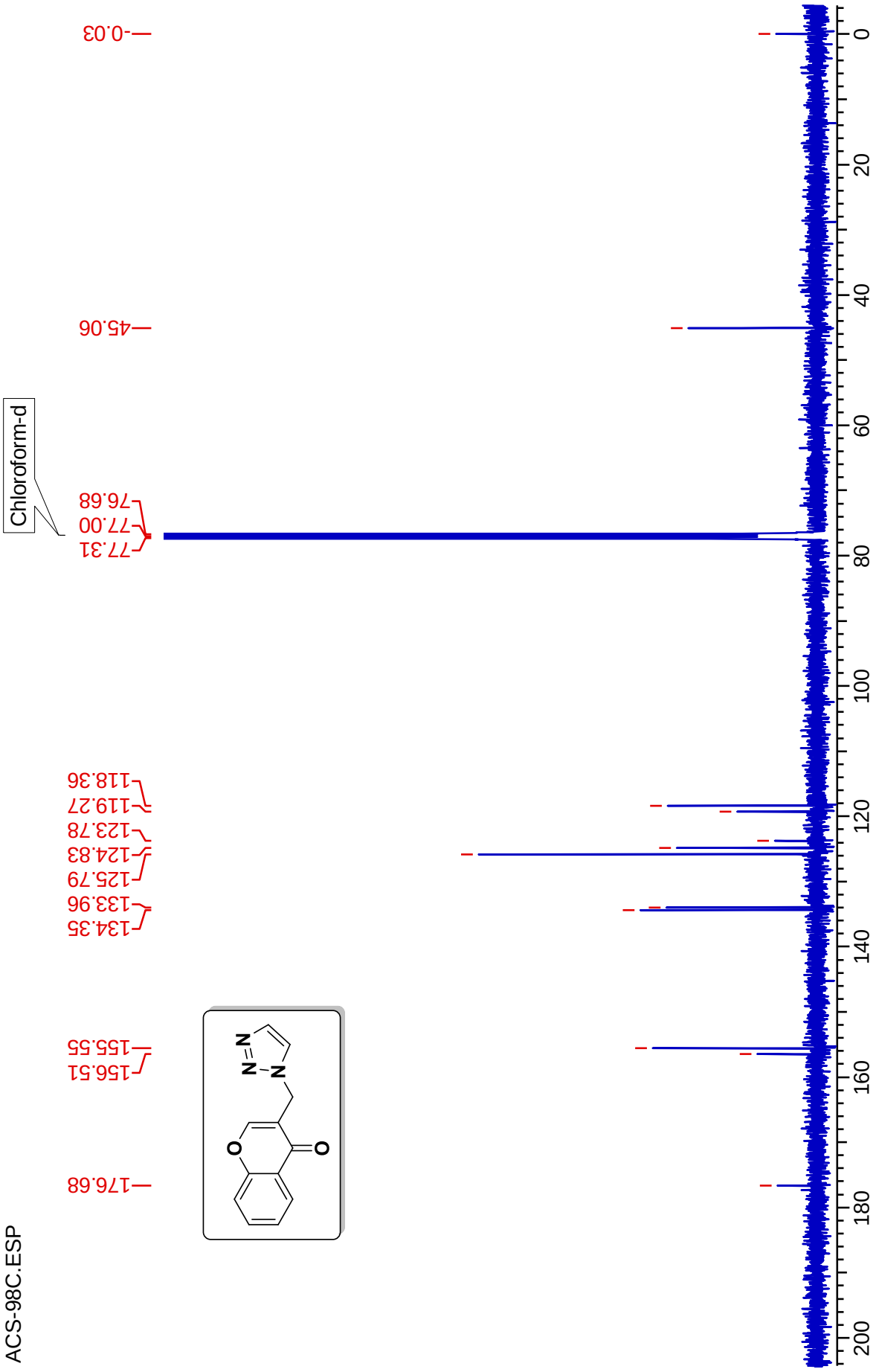
HRMS of compound ***6s***:



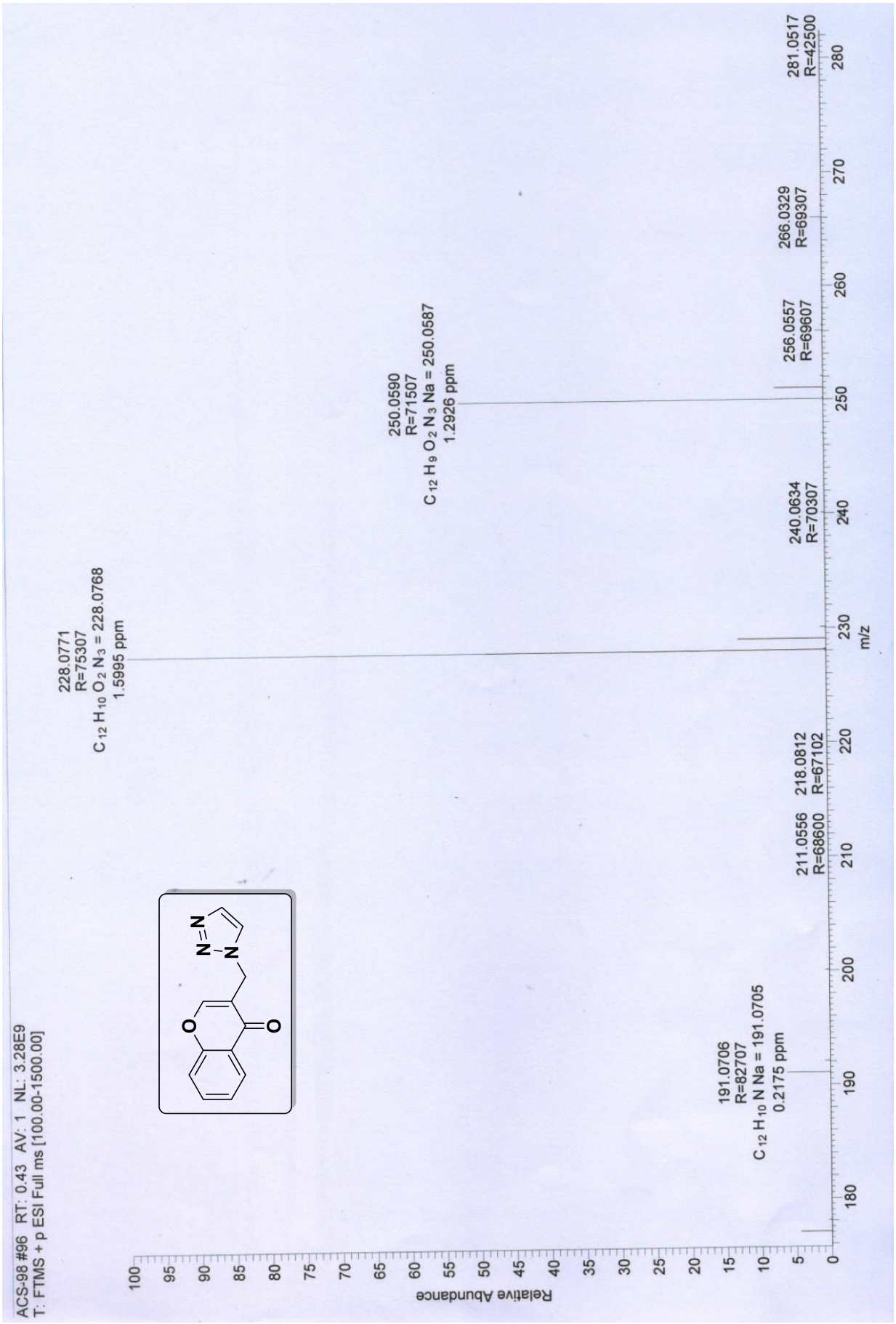
^{1}H NMR (400 MHz, $CDCl_3$) of compound ***6t***:



^{13}C NMR (100 MHz, $CDCl_3$) of compound ***6t***:



HRMS of compound ***6t***:



***In-vitro* MTB MABA assay**

Briefly, the inoculum was prepared from fresh LJ medium re-suspended in 7H9-S medium (7H9 broth, 0.1% casitone, 0.5% glycerol, supplemented oleic acid, albumin, dextrose, and catalase [OADC]), adjusted to a McFarland tube No. 1, and diluted 1:20; 100 µl was used as inoculum. Each drug stock solution was thawed and diluted in 7H9-S at four-fold the final highest concentration tested. Serial two-fold dilutions of each drug were prepared directly in a sterile 96-well microtiter plate using 100 µl 7H9-S. A growth control containing no antibiotic and a sterile control were also prepared on each plate. Sterile water was added to all perimetre wells to avoid evaporation during the incubation. The plate was covered, sealed in plastic bags and incubated at 37ºC in normal atmosphere. After 7 days incubation, 30 ml of alamar blue solution was added to each well, and the plate was re-incubated overnight. A change in colour from blue (oxidised state) to pink (reduced) indicated the growth of bacteria, and the MIC was defined as the lowest concentration of drug that prevented this change in colour.

***In-vitro* cytotoxicity screening**

Some compounds were further examined for toxicity in a RAW 264.7 cell line at the concentration of 50 µM. After 72 h of exposure, viability was assessed on the basis of cellular conversion of MTT into a formazan product using the Promega Cell Titer 96 non-radioactive cell proliferation assay.

	MIC in µM
Rifampicin	0.24
Ethambutol	7.64

Correlation of bioactivity with respect to GLIDE Score Binding Energy (kcal/mol) of 1ZID (Enoyl-acyl carrier protein)

Figure:

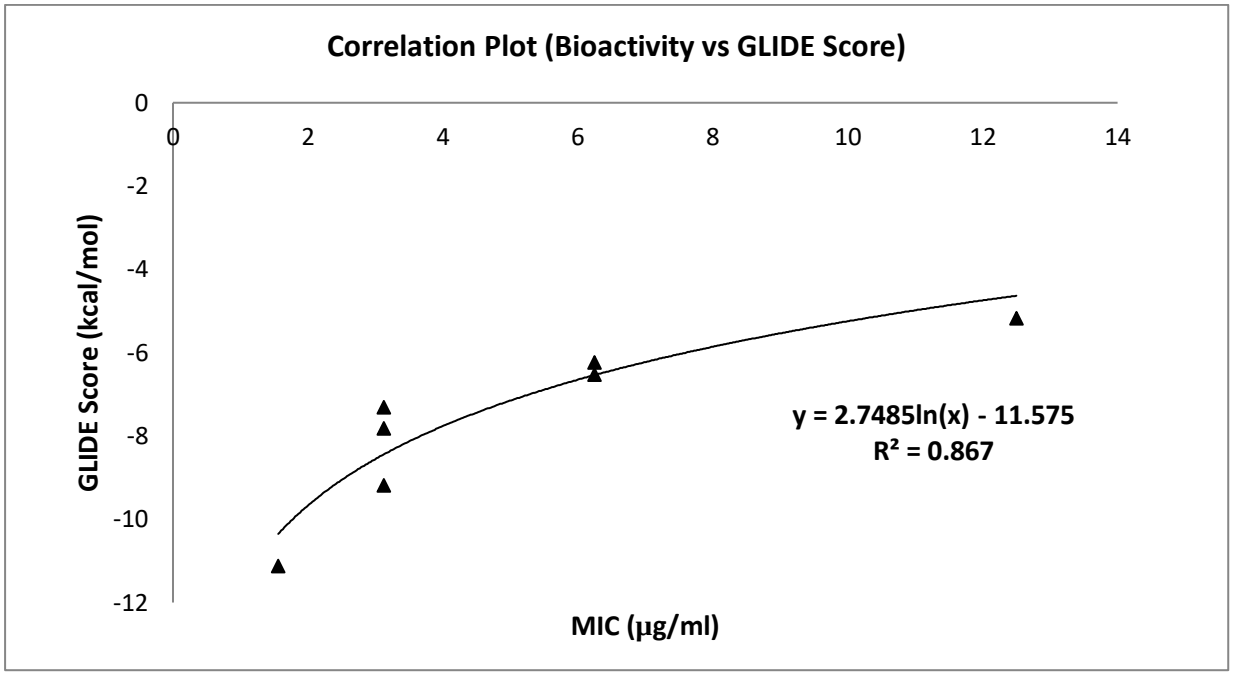


Table: In vitro anti-tubercular activity MIC (µg/ml) and GLIDE Score (kcal/mol)

Compound	MIC (µg/ml)	GLIDE Score (BE)
6s	1.56	-11.123
6h	3.125	-9.189
6f	3.125	-7.826
6o	3.125	-7.316
6m	6.25	-6.525
6g	6.25	-6.238
6p	12.5	-5.176