

Supporting Information

For

Selective synthesis of *N*-[1,3,5]Triazinyl- α -ketoamides and

***N*-[1,3,5]Triazinyl-amides from the reactions of**

2-amine-[1,3,5]triazines with ketones

Yue Li, Pengzhen Zhong, Junna Zhao, Zexi Pan, Chen Zhang, and Dongmei Cui

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_210507_pzc_2_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_210507_pzc_2_0m

Bond precision:	C-C = 0.0016 A	Wavelength=0.71073
Cell:	a=7.6548(2)	b=12.1882(3) c=14.4395(4)
	alpha=90	beta=103.691(1) gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	1308.90(6)	1308.90(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H13 N5 O2	C13 H13 N5 O2
Sum formula	C13 H13 N5 O2	C13 H13 N5 O2
Mr	271.28	271.28
Dx,g cm-3	1.377	1.377
Z	4	4
Mu (mm-1)	0.098	0.098
F000	568.0	568.0
F000'	568.22	
h,k,lmax	9,15,18	9,15,18
Nref	2895	2894
Tmin,Tmax	0.957,0.966	0.687,0.746
Tmin'	0.957	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.099

R(reflections)= 0.0356(2569) wR2(reflections)= 0.0989(2894)

S = 1.066 Npar= 183

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.



Alert level C

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C7 - C8 . 1.53 Ang.



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
 PLAT432_ALERT_2_G Short Inter X...Y Contact C5 ..C5 3.15 Ang.
 1-x,1-y,2-z = 3_667 Check
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
 PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
 0 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

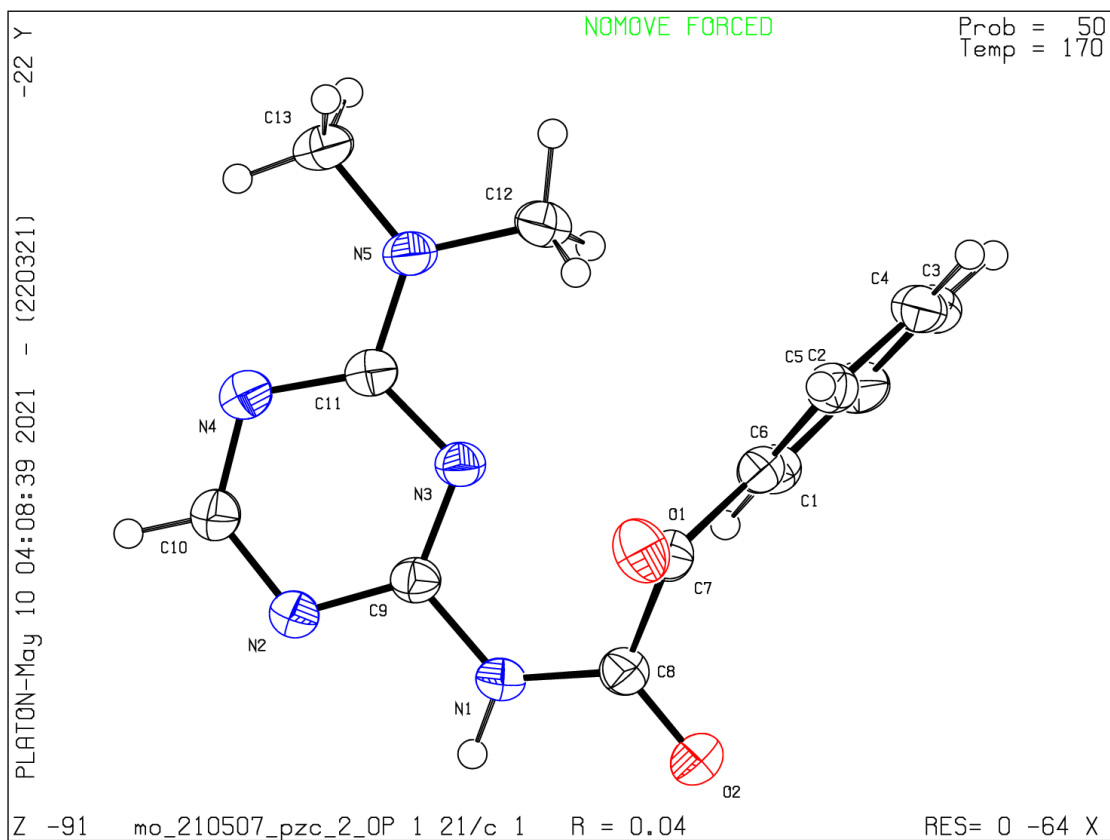
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

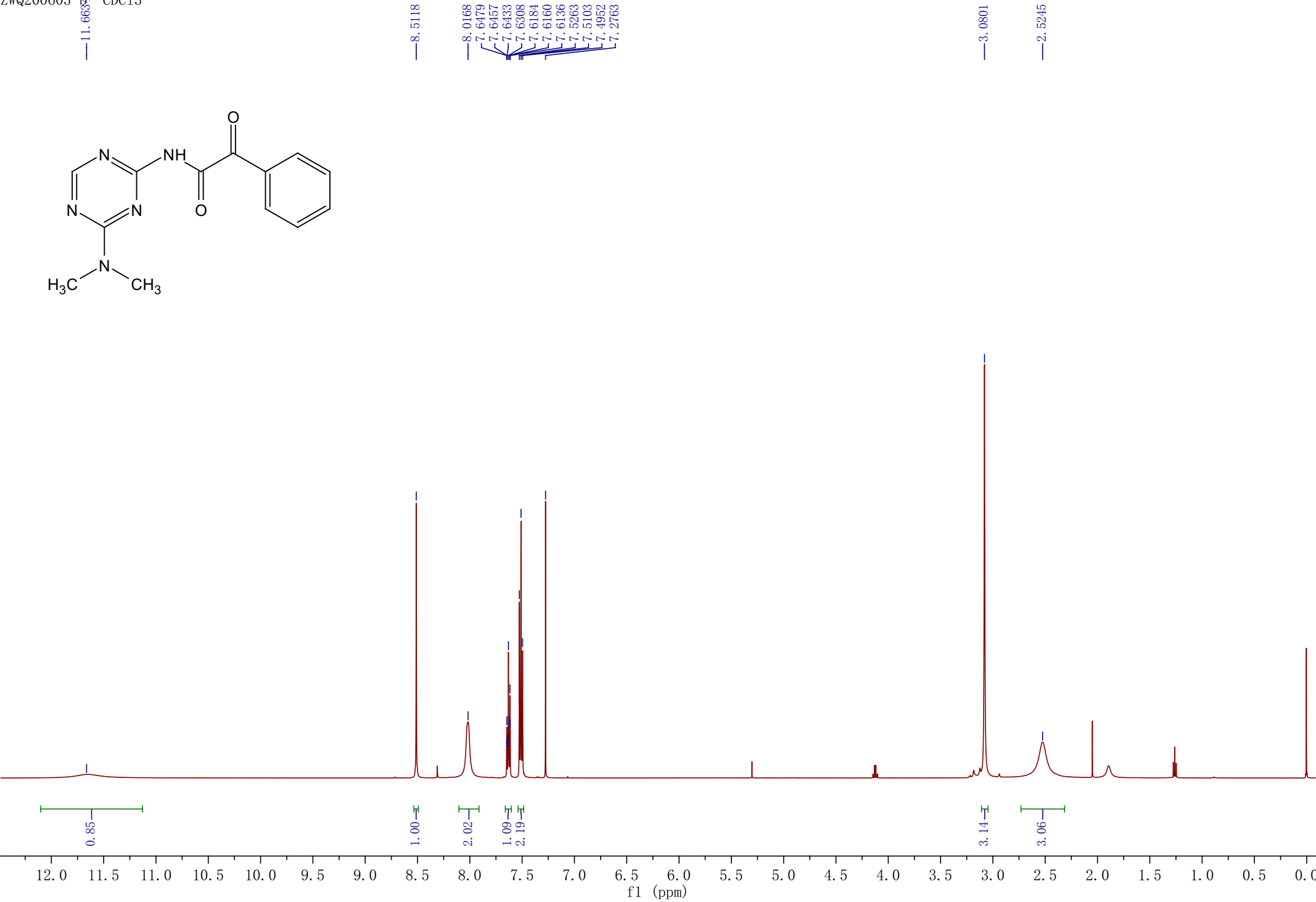
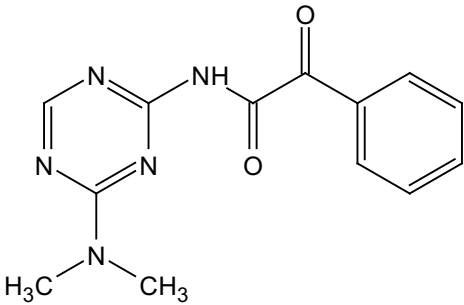
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

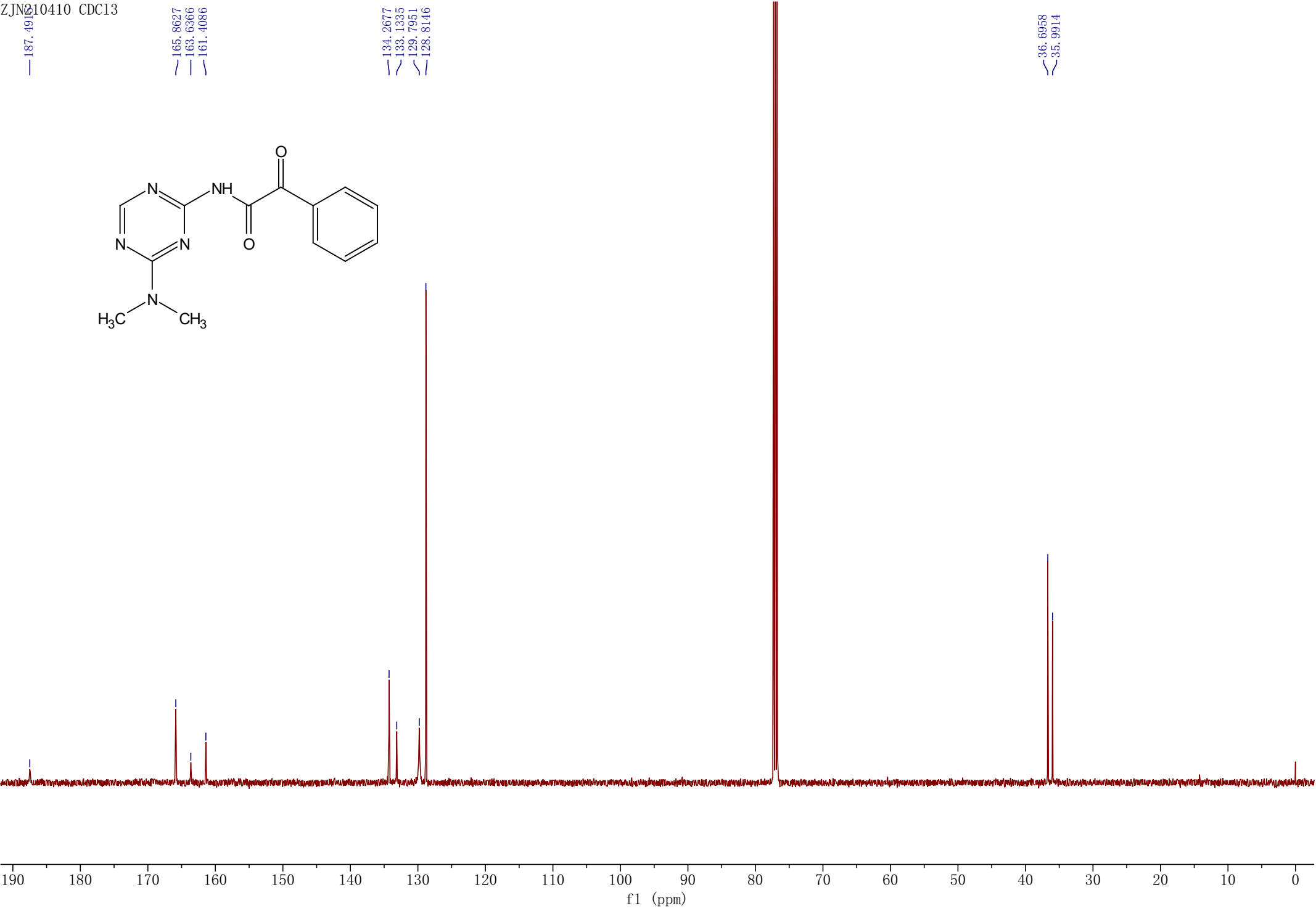
Publication of your CIF in other journals

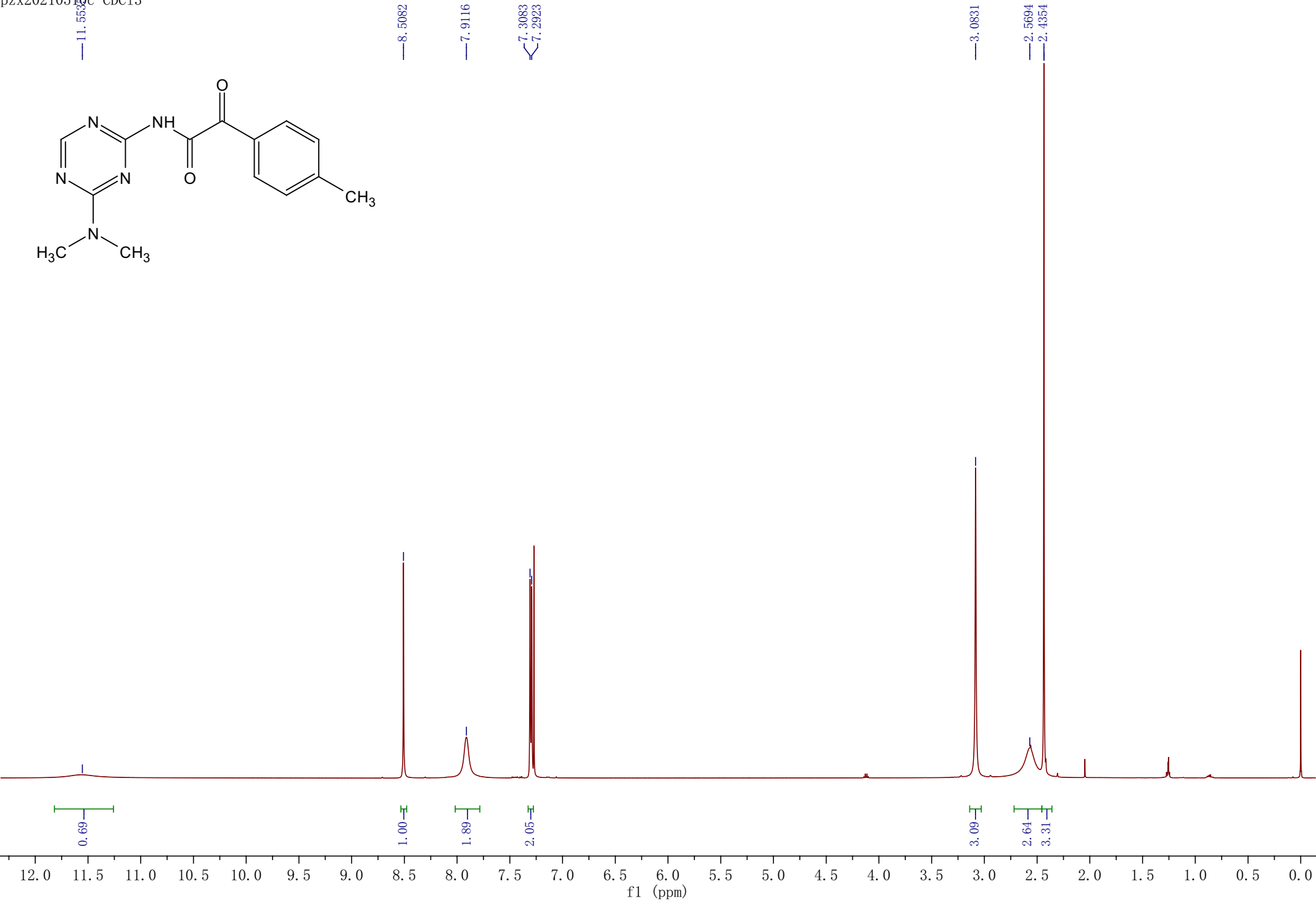
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.



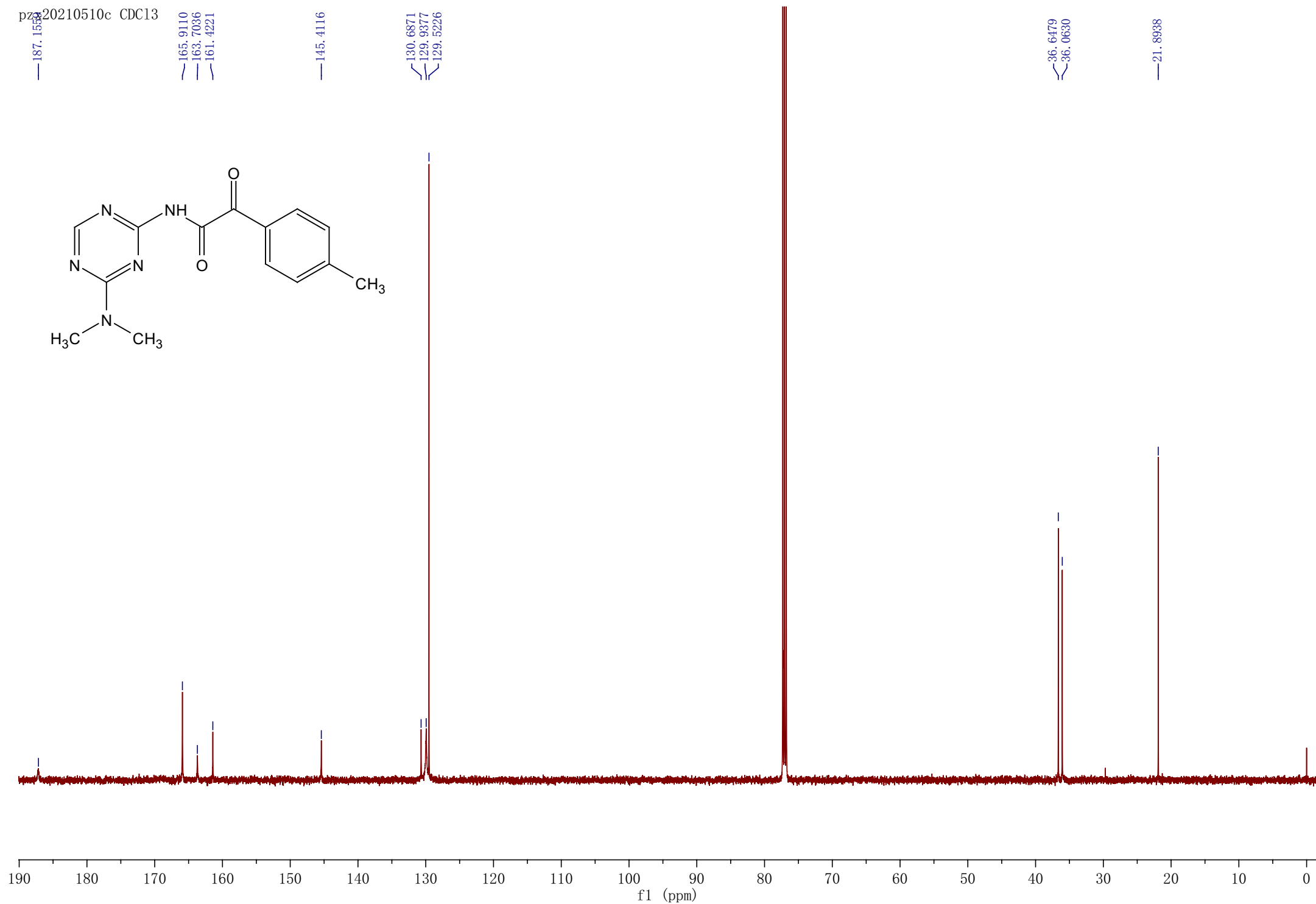
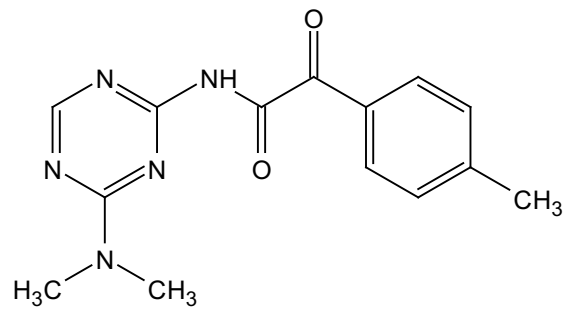


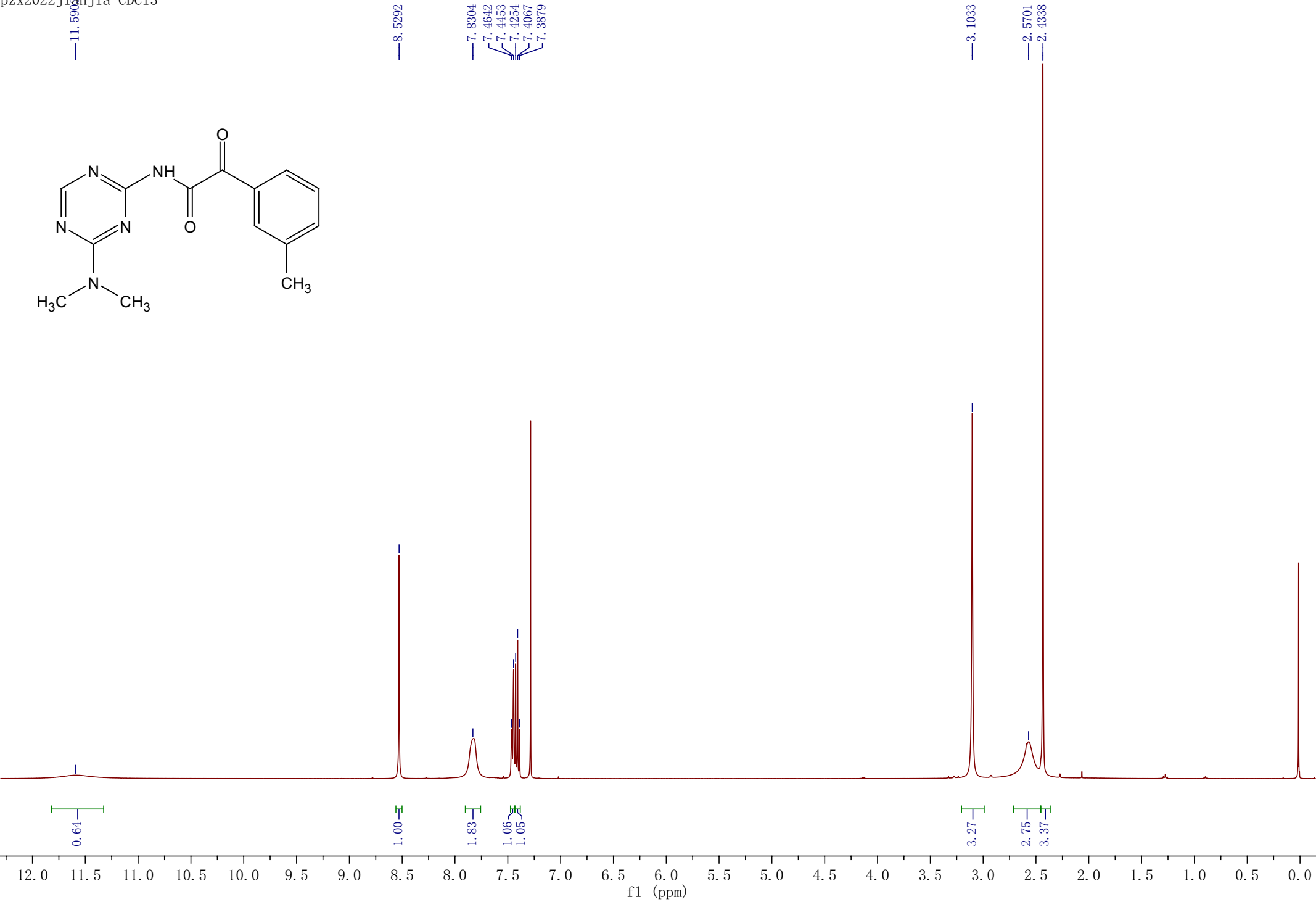
ZJN210410 CDC13



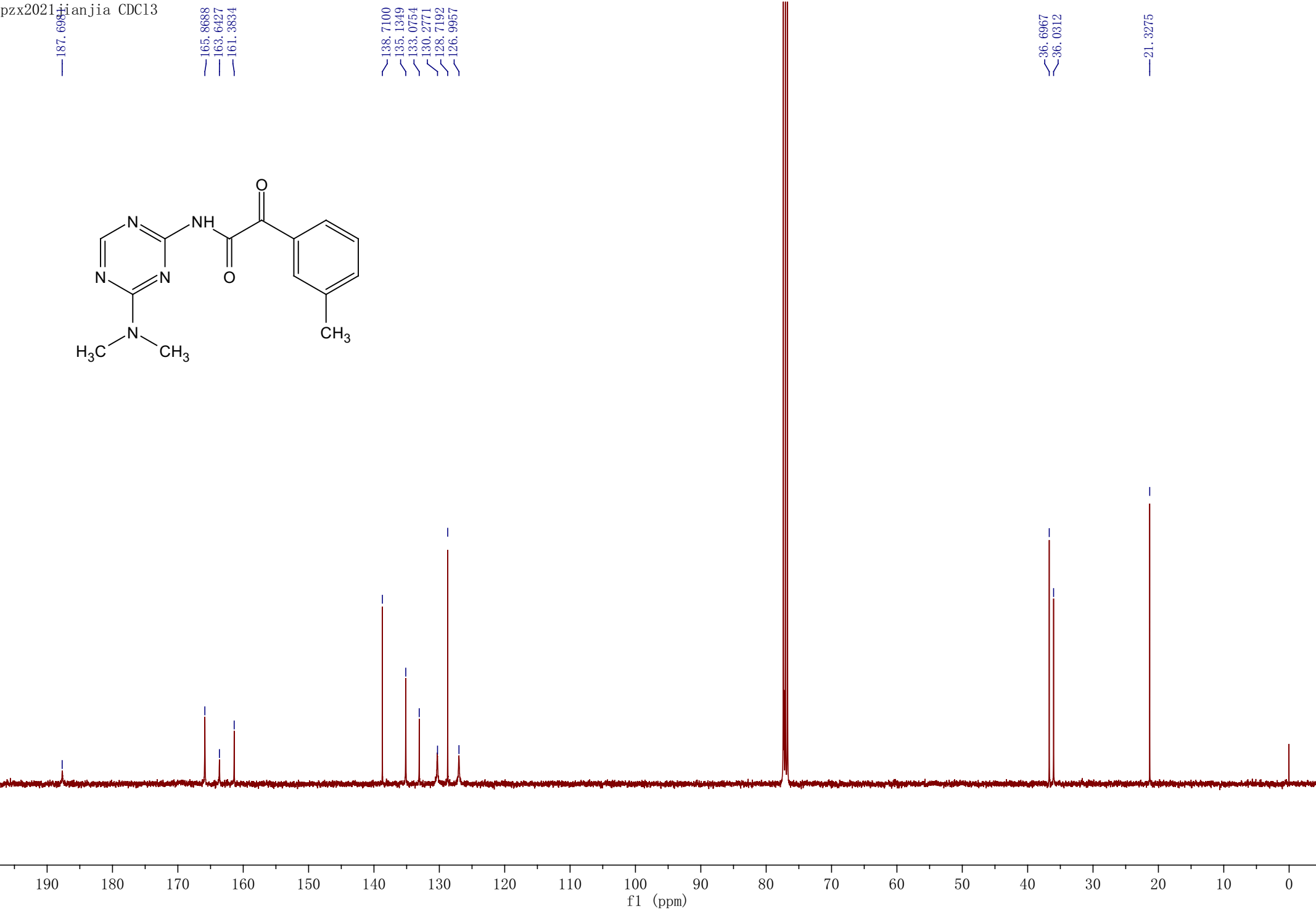


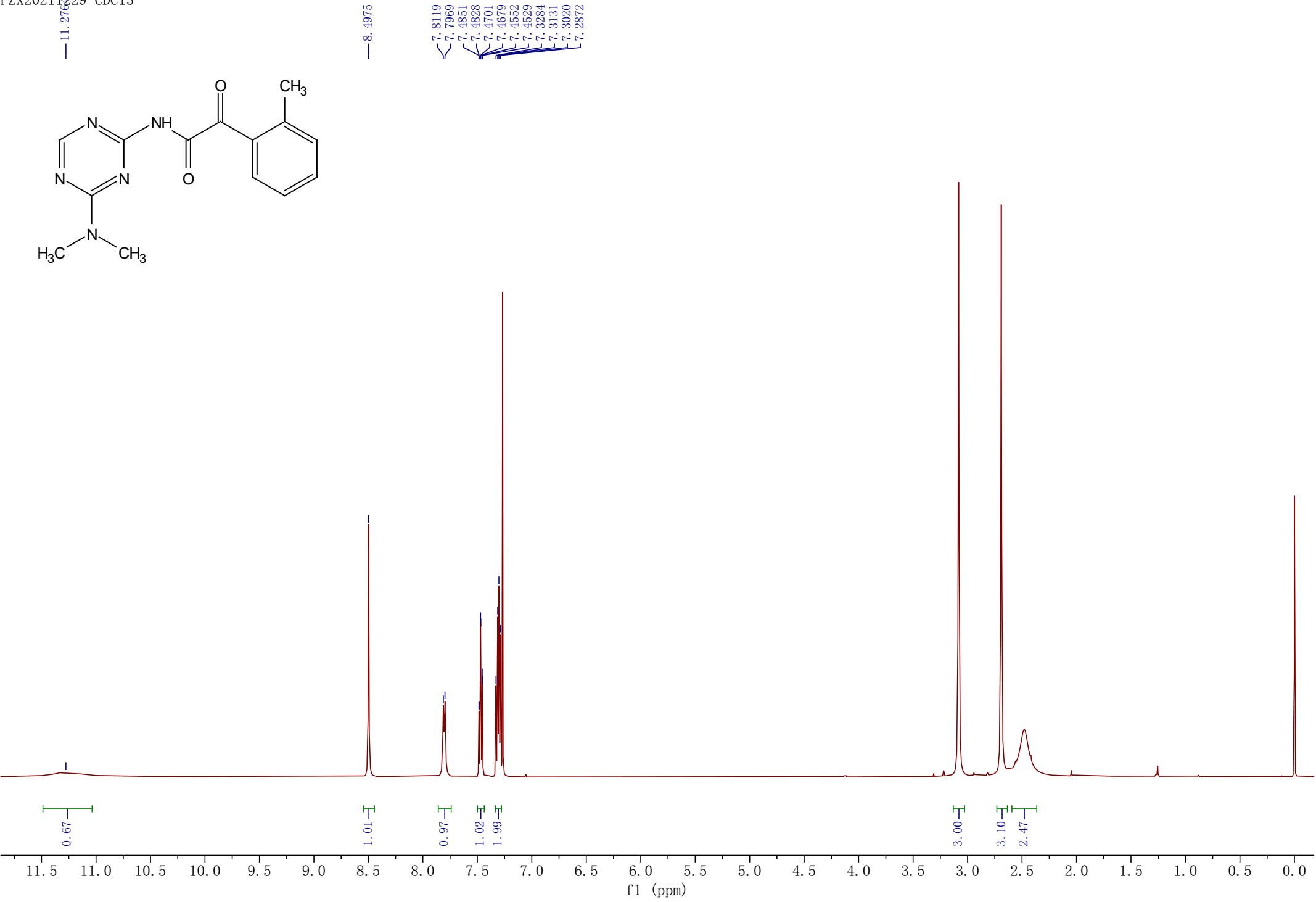
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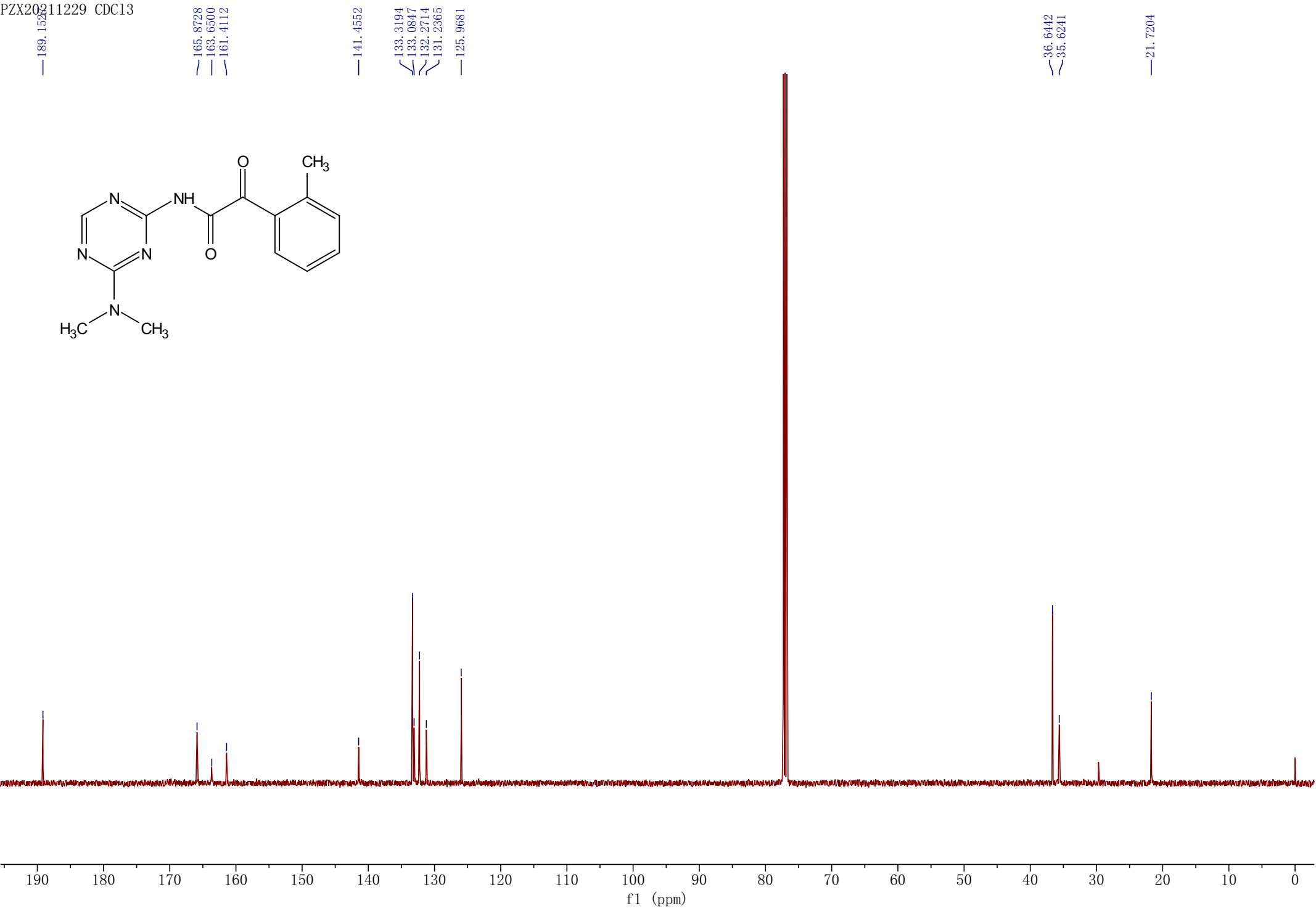
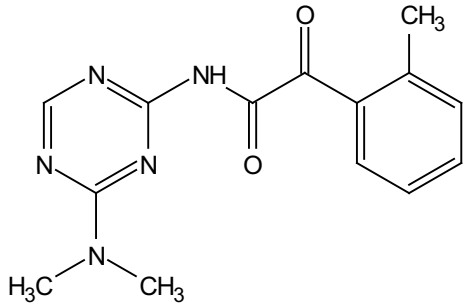


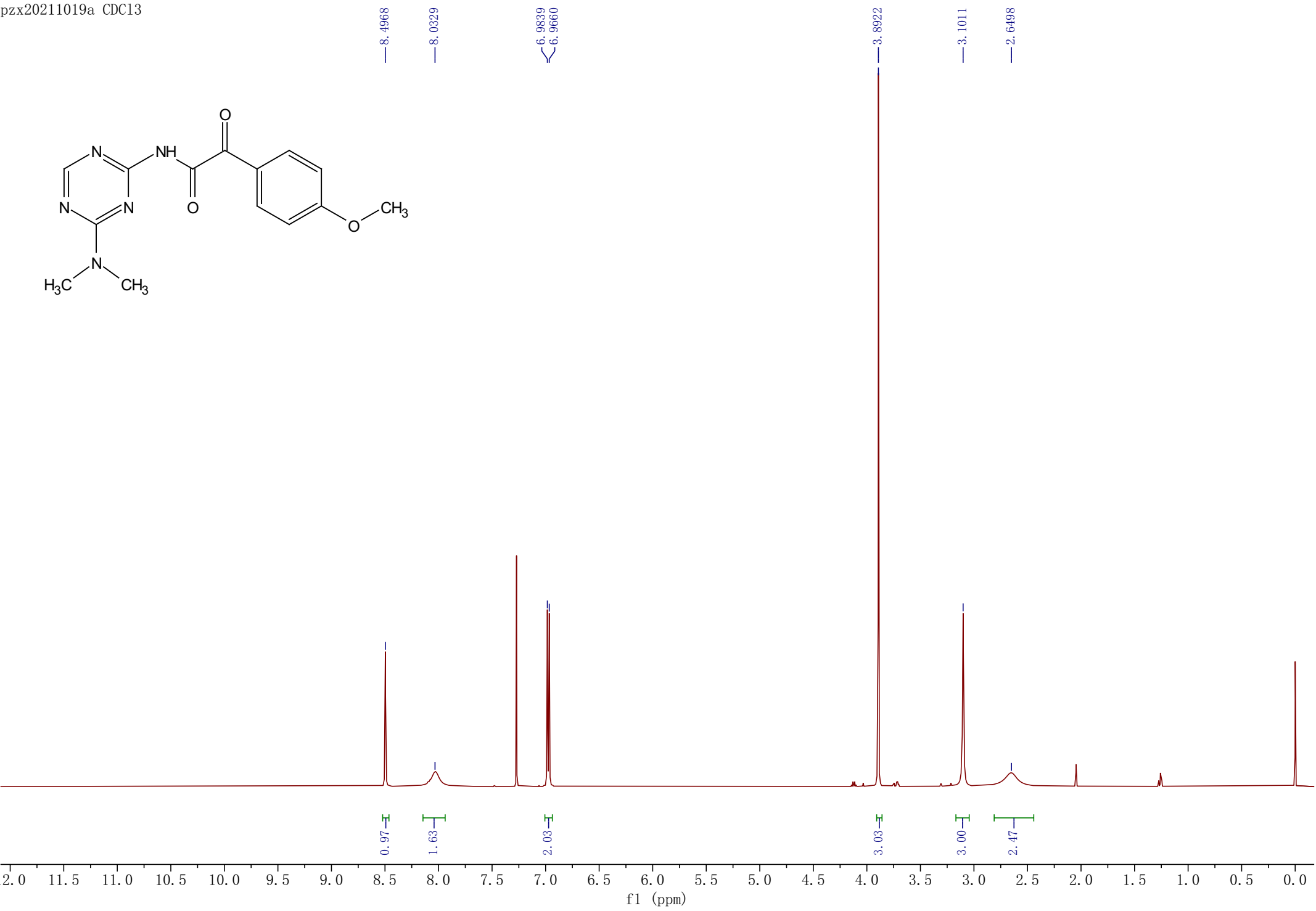
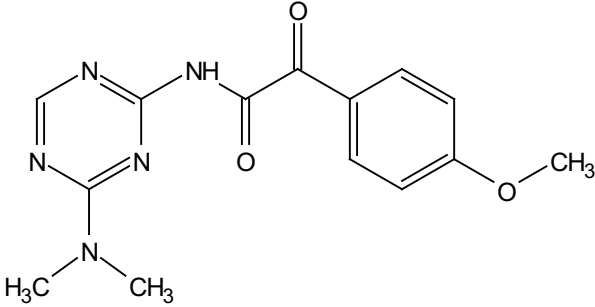


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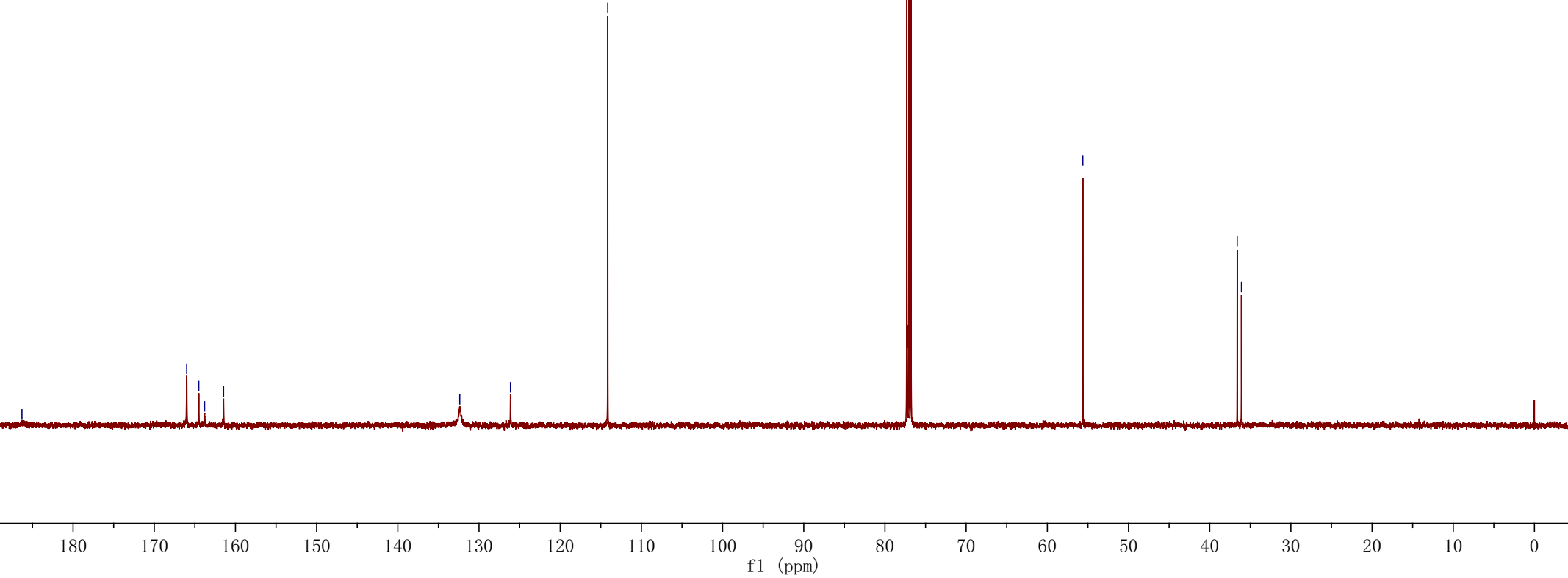
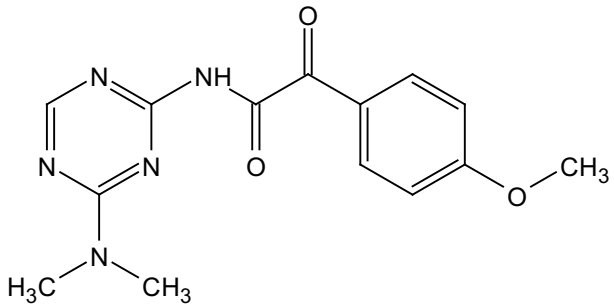


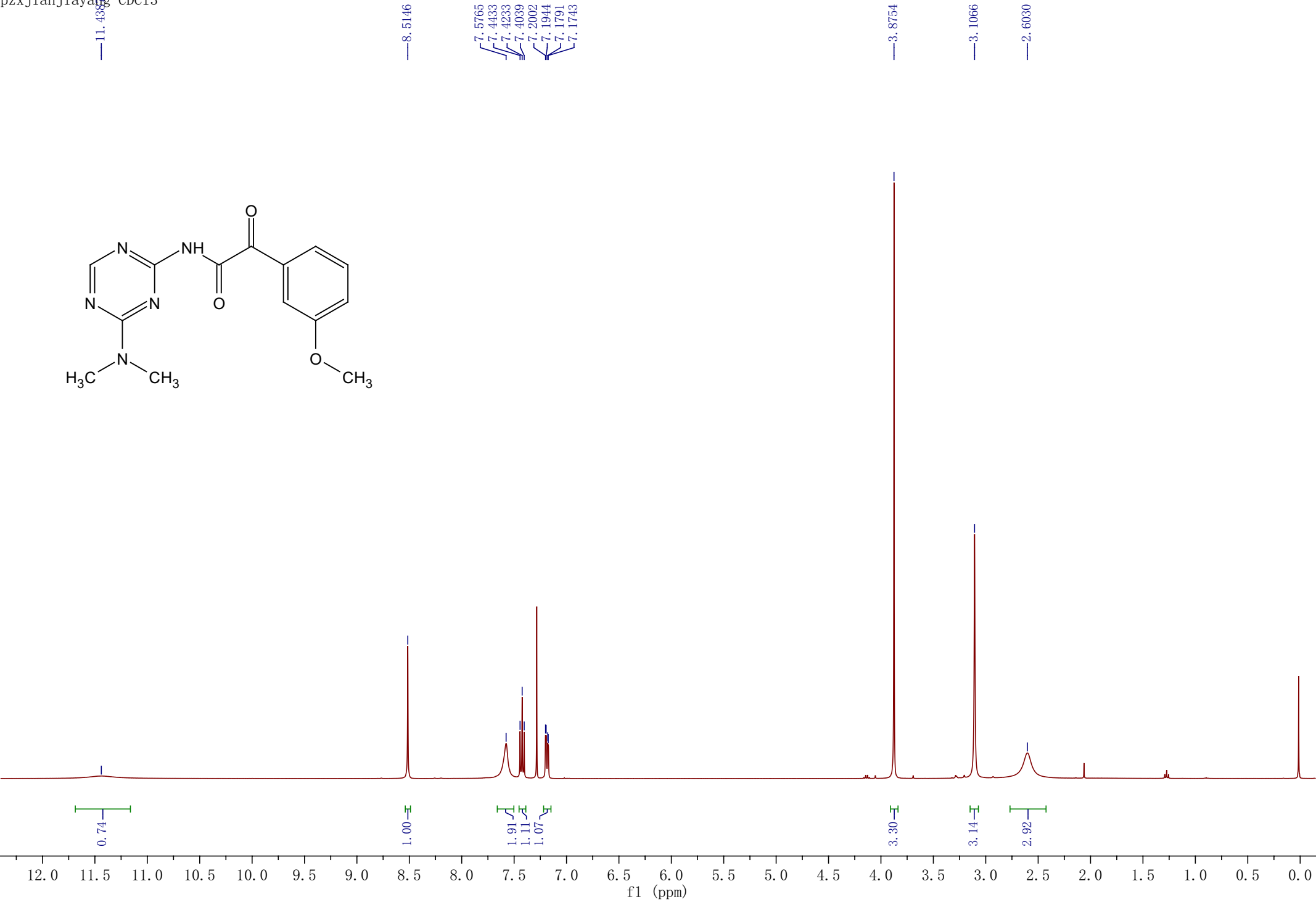




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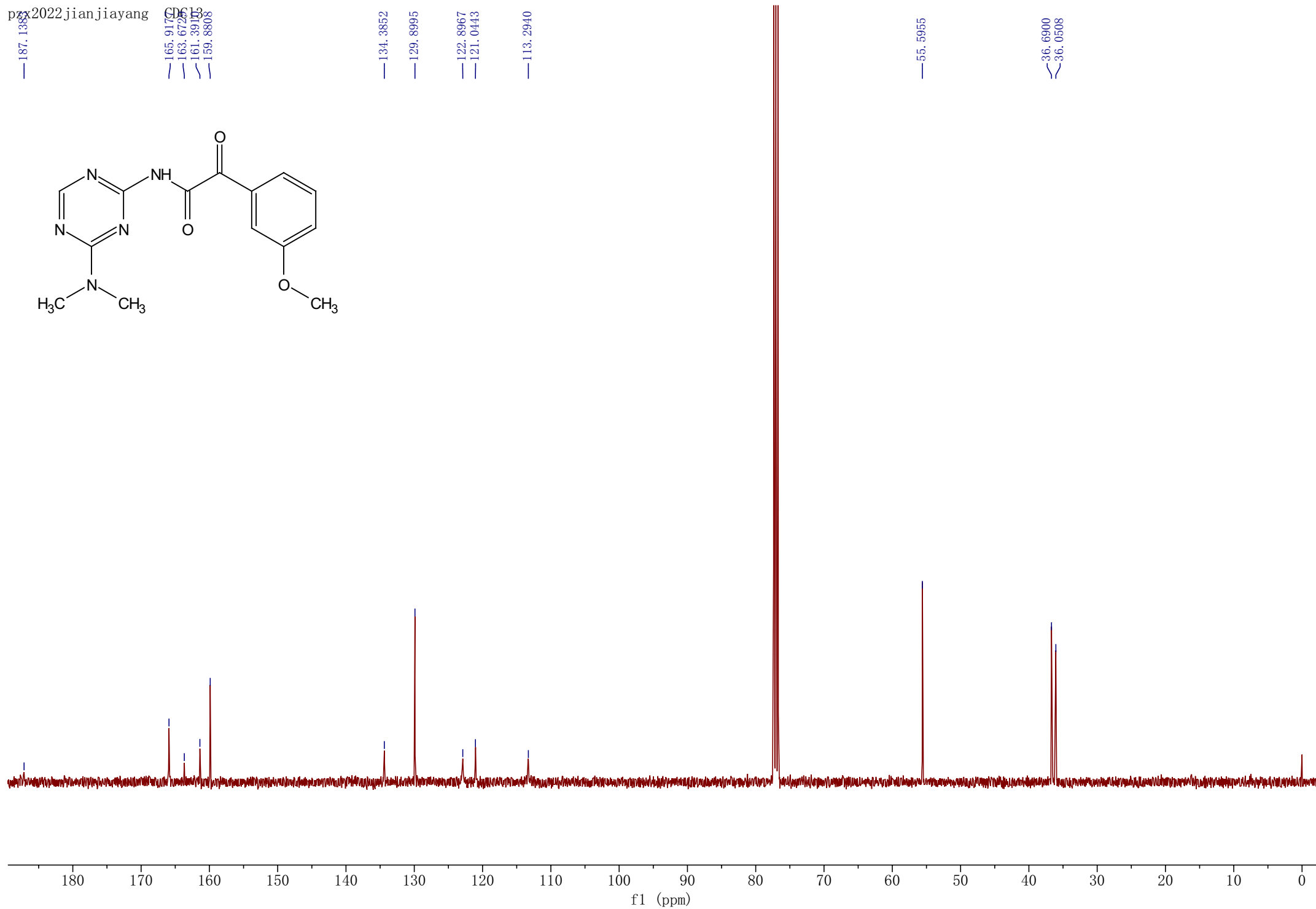
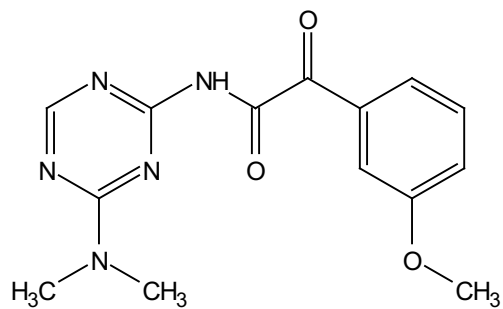
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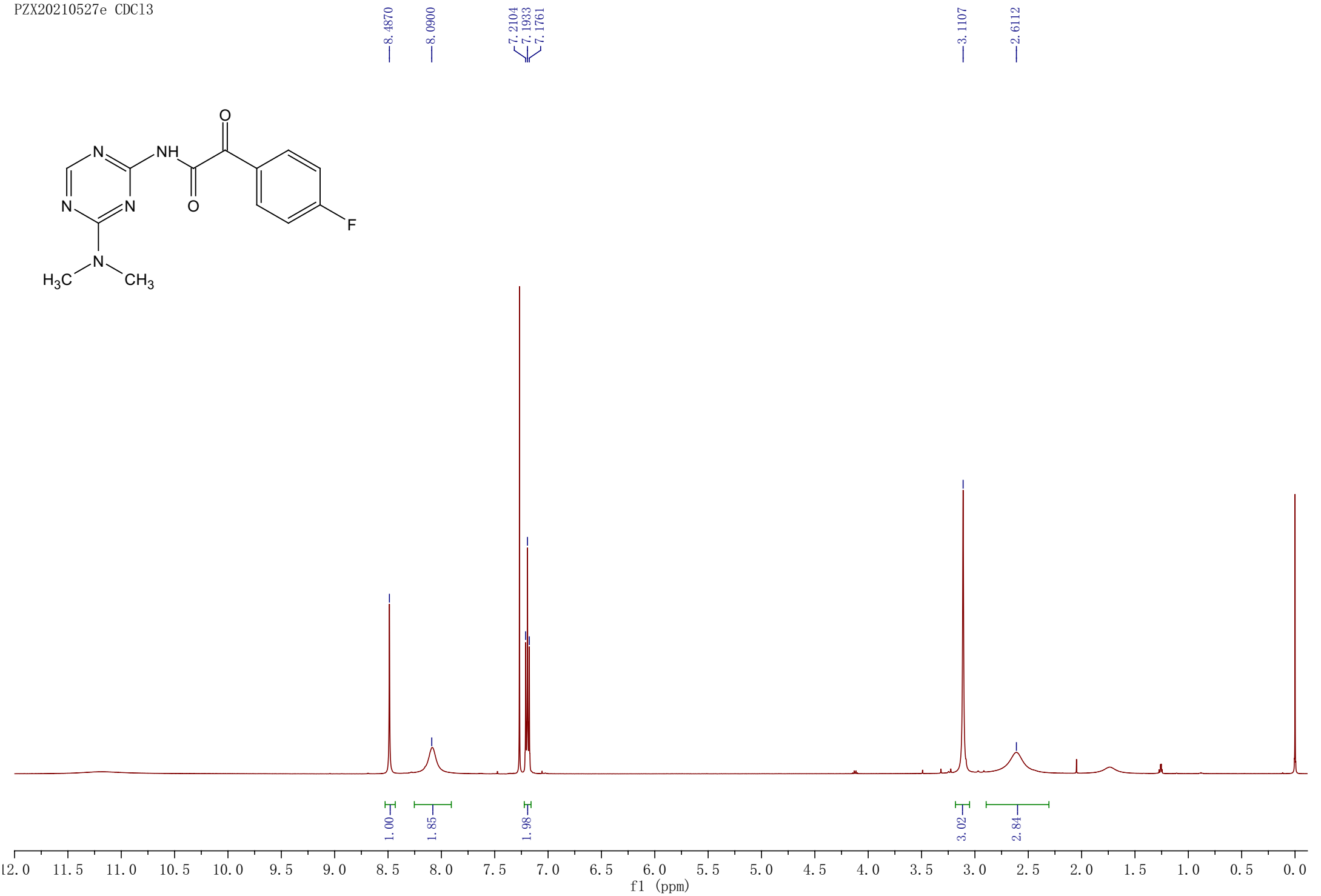
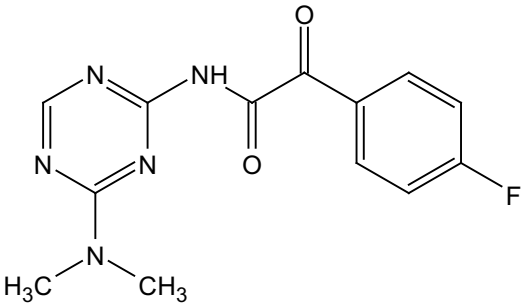




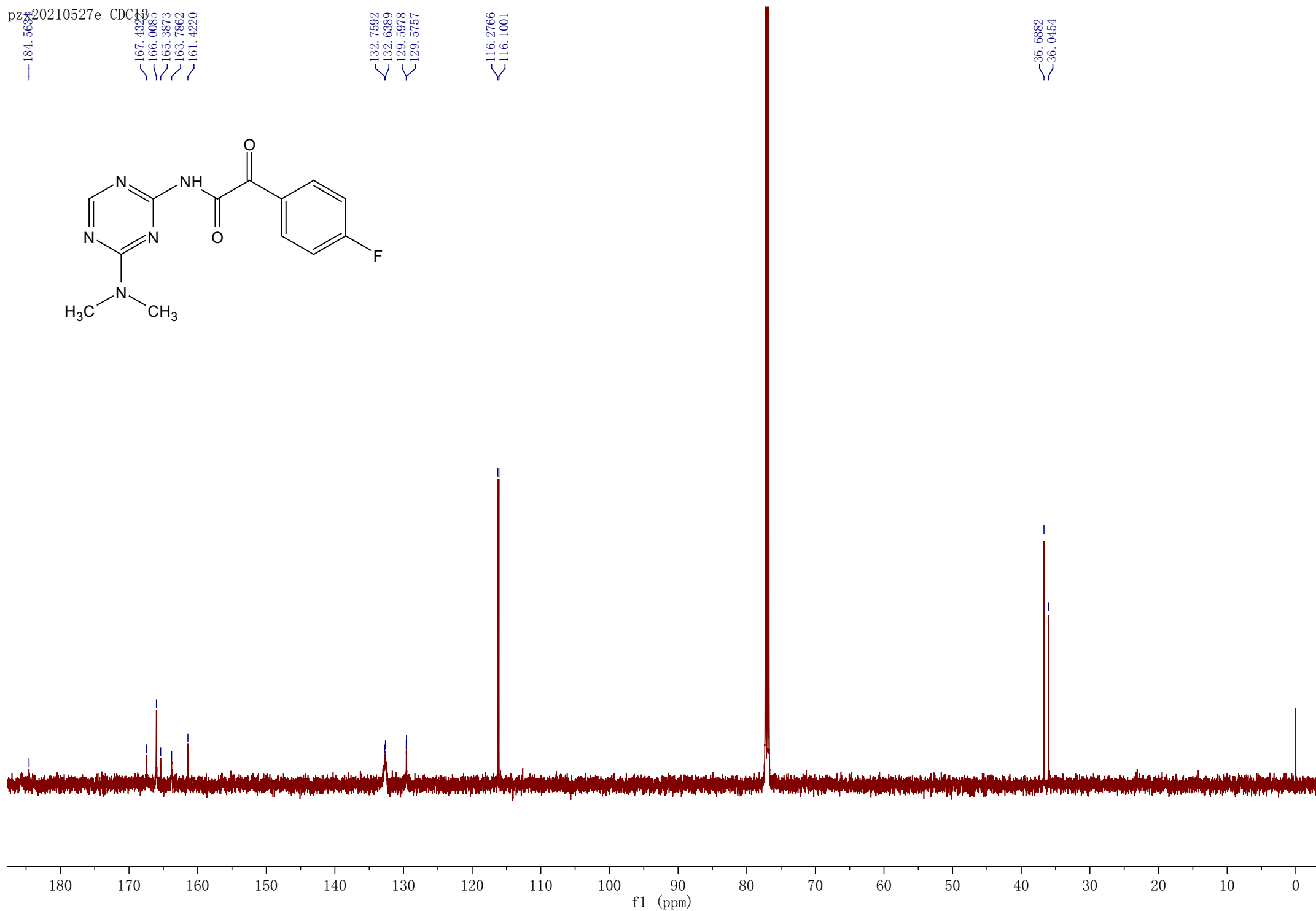
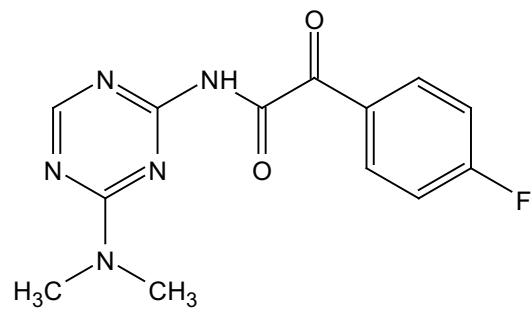
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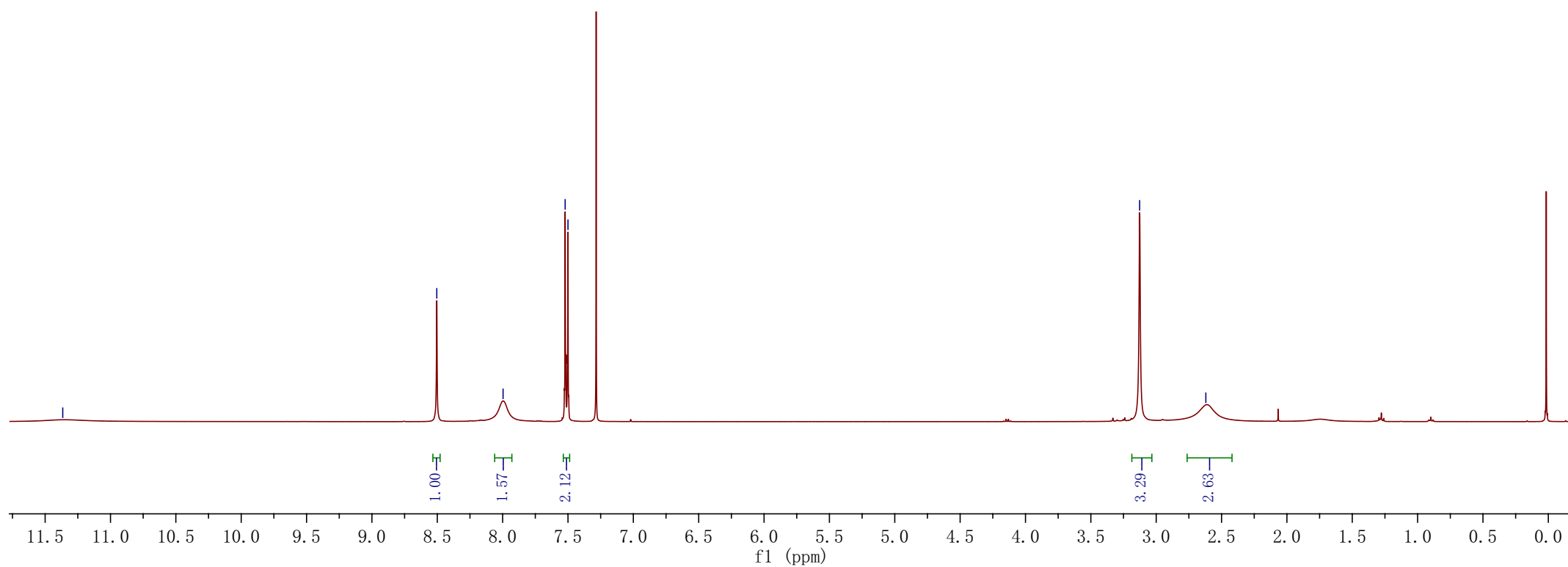
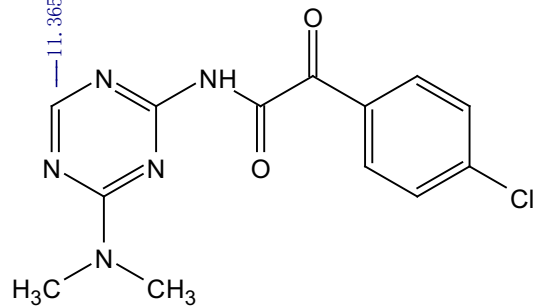




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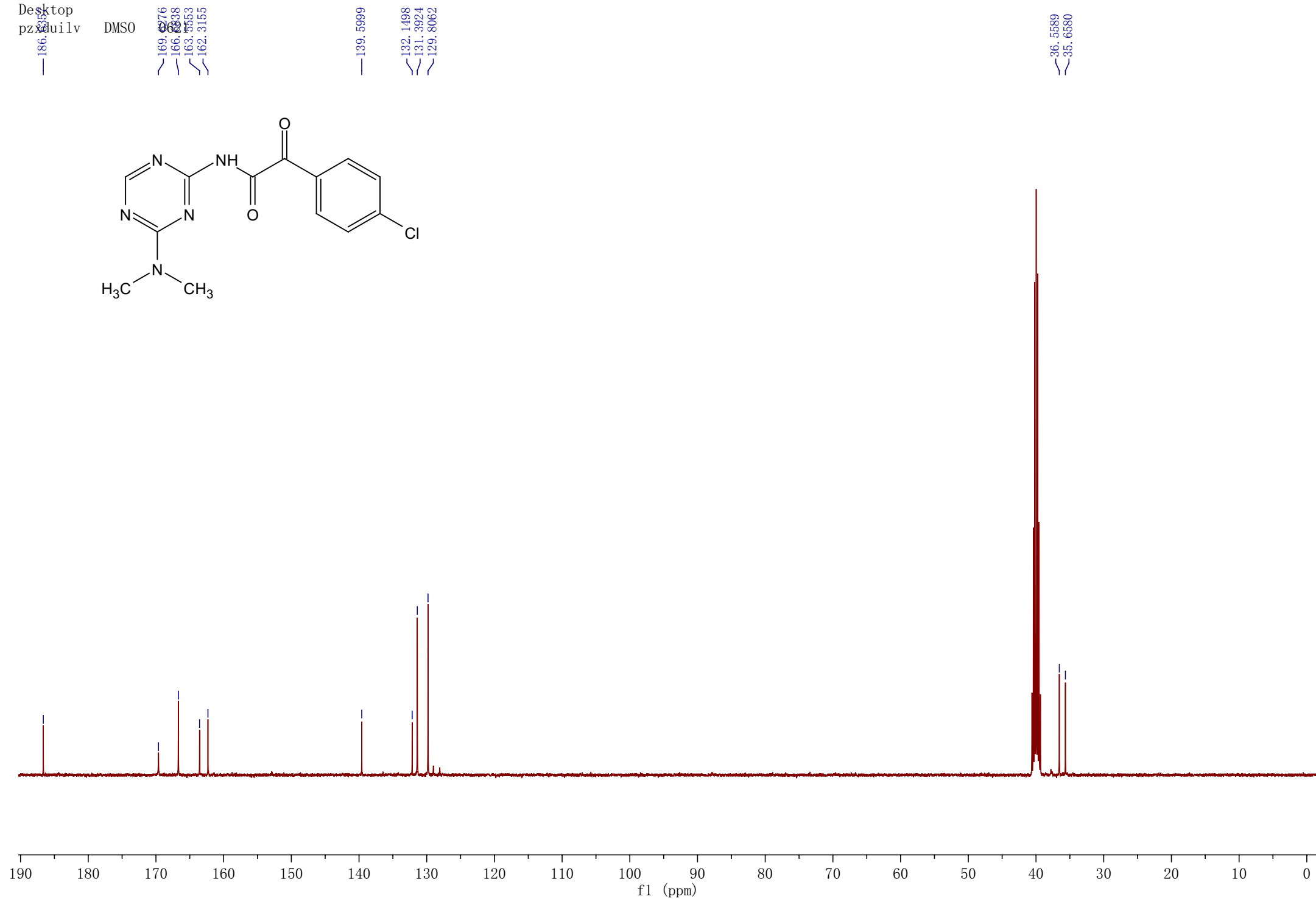
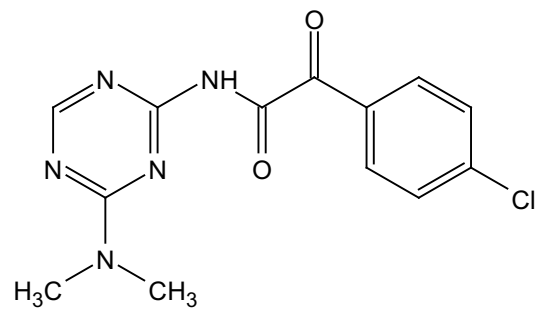


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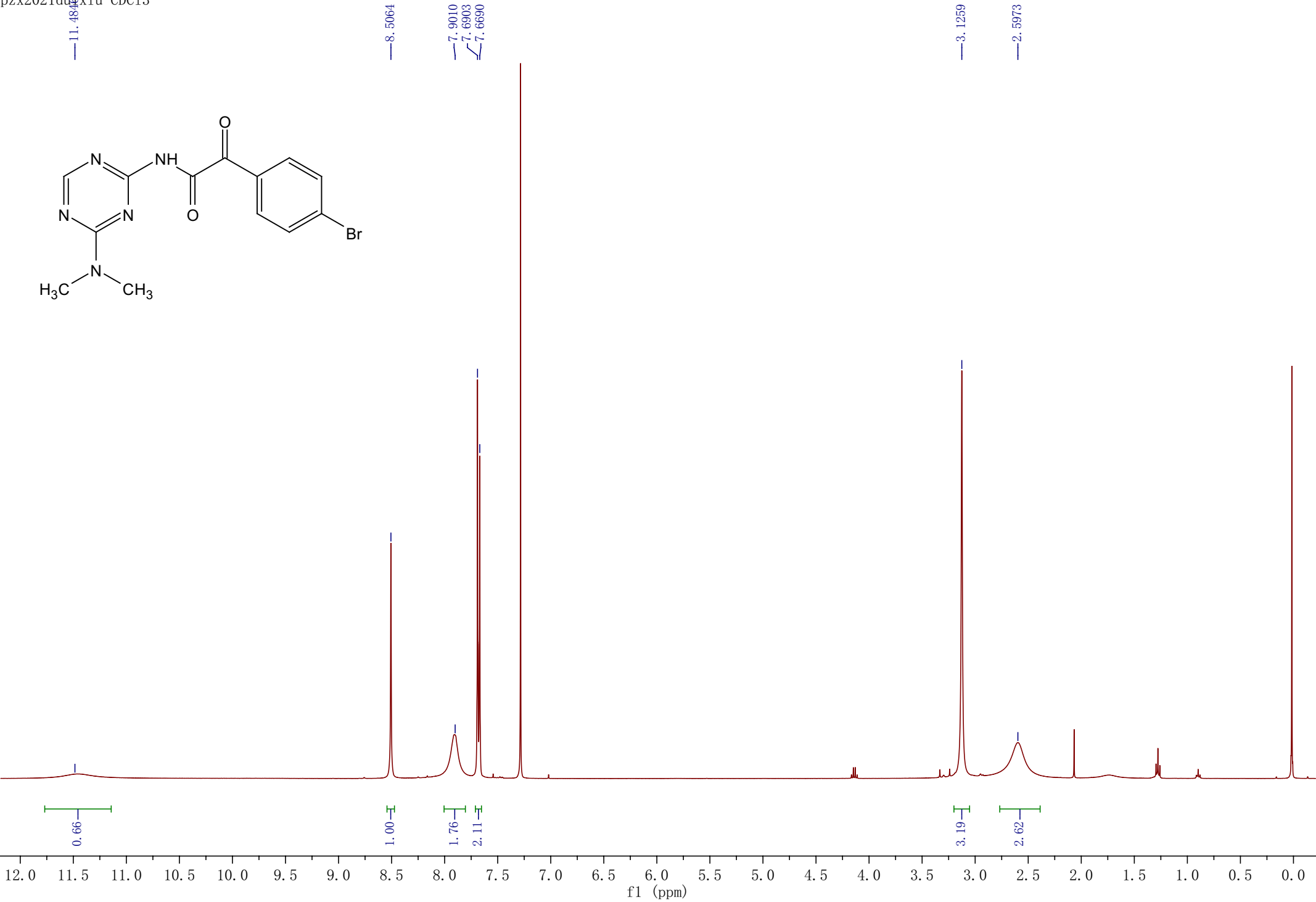


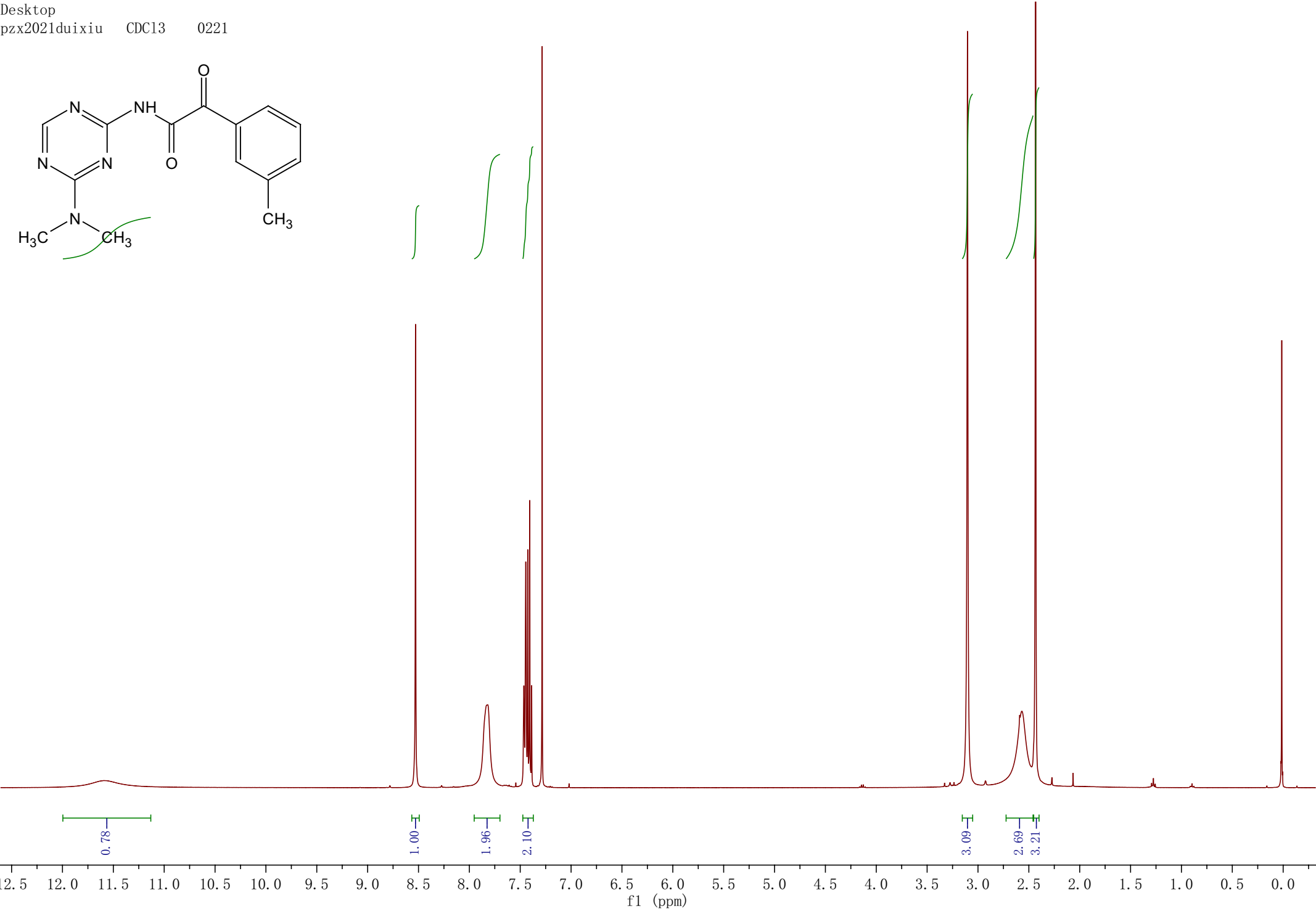
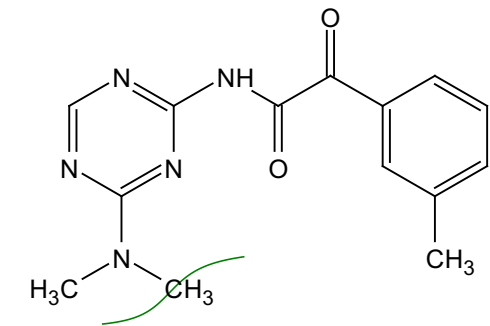
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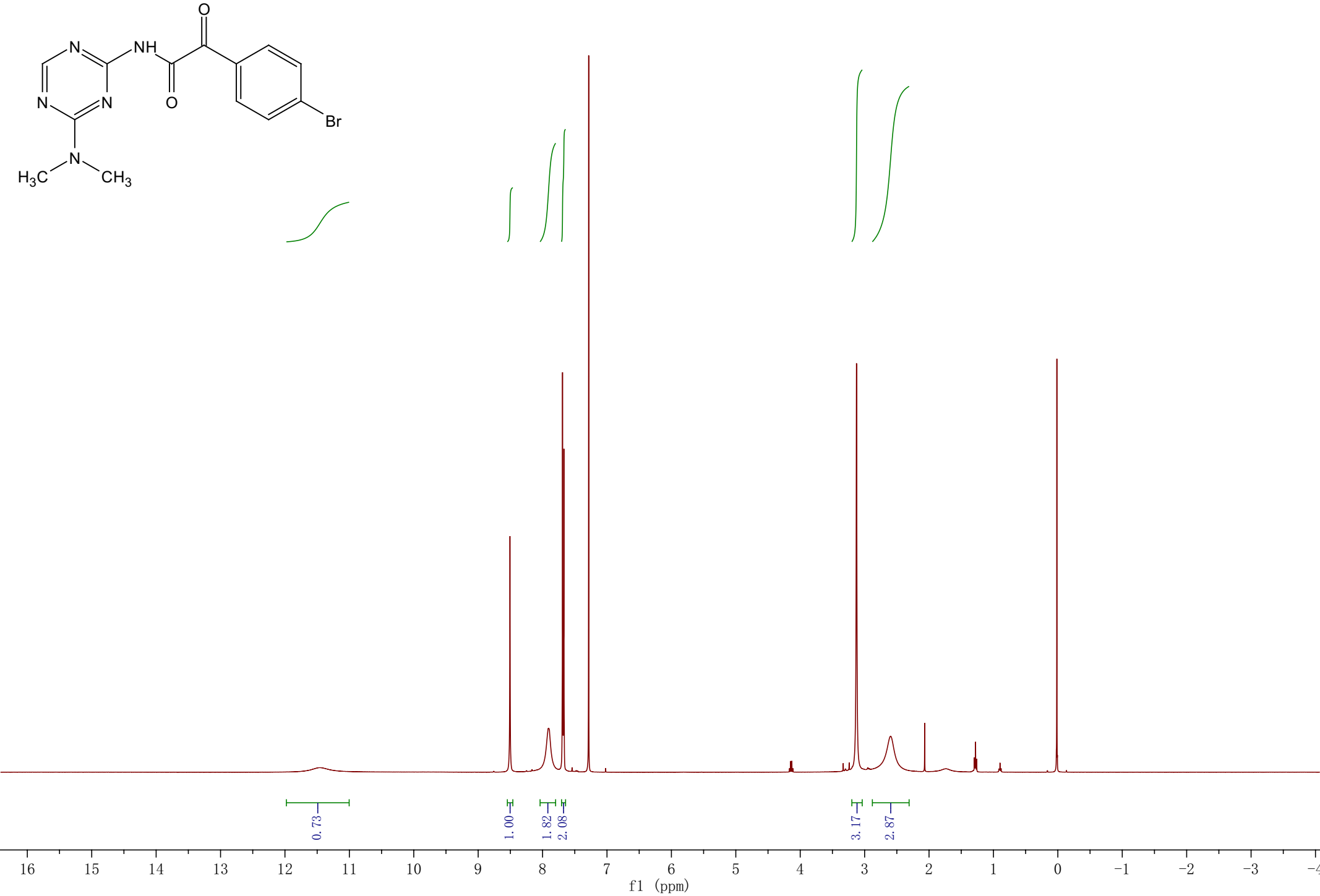
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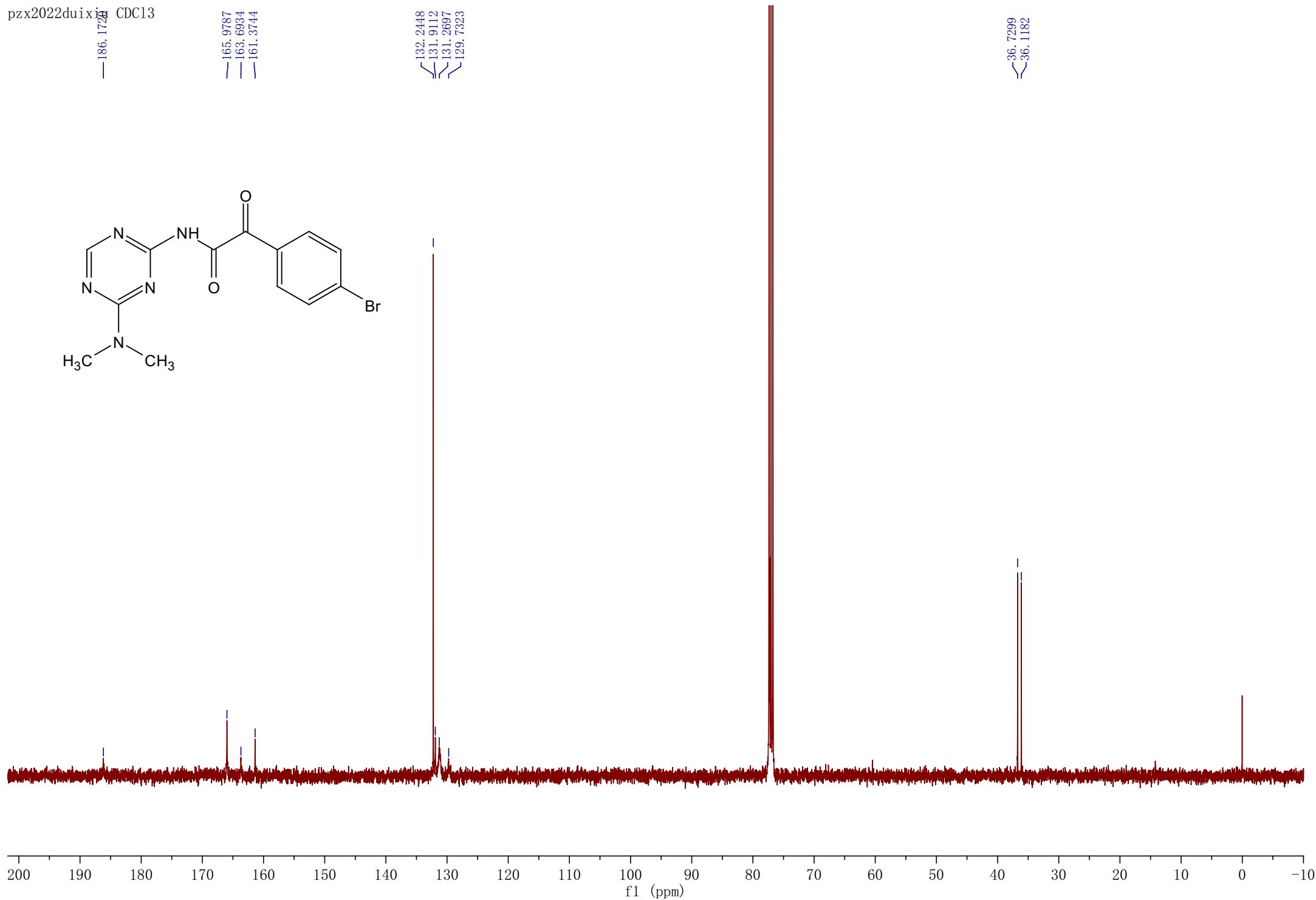
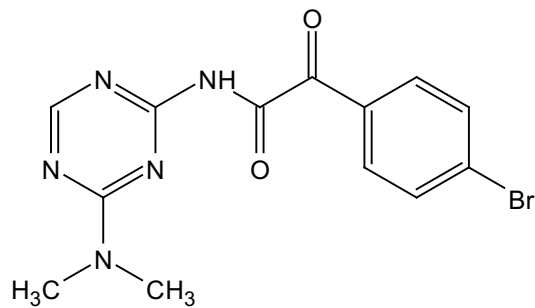
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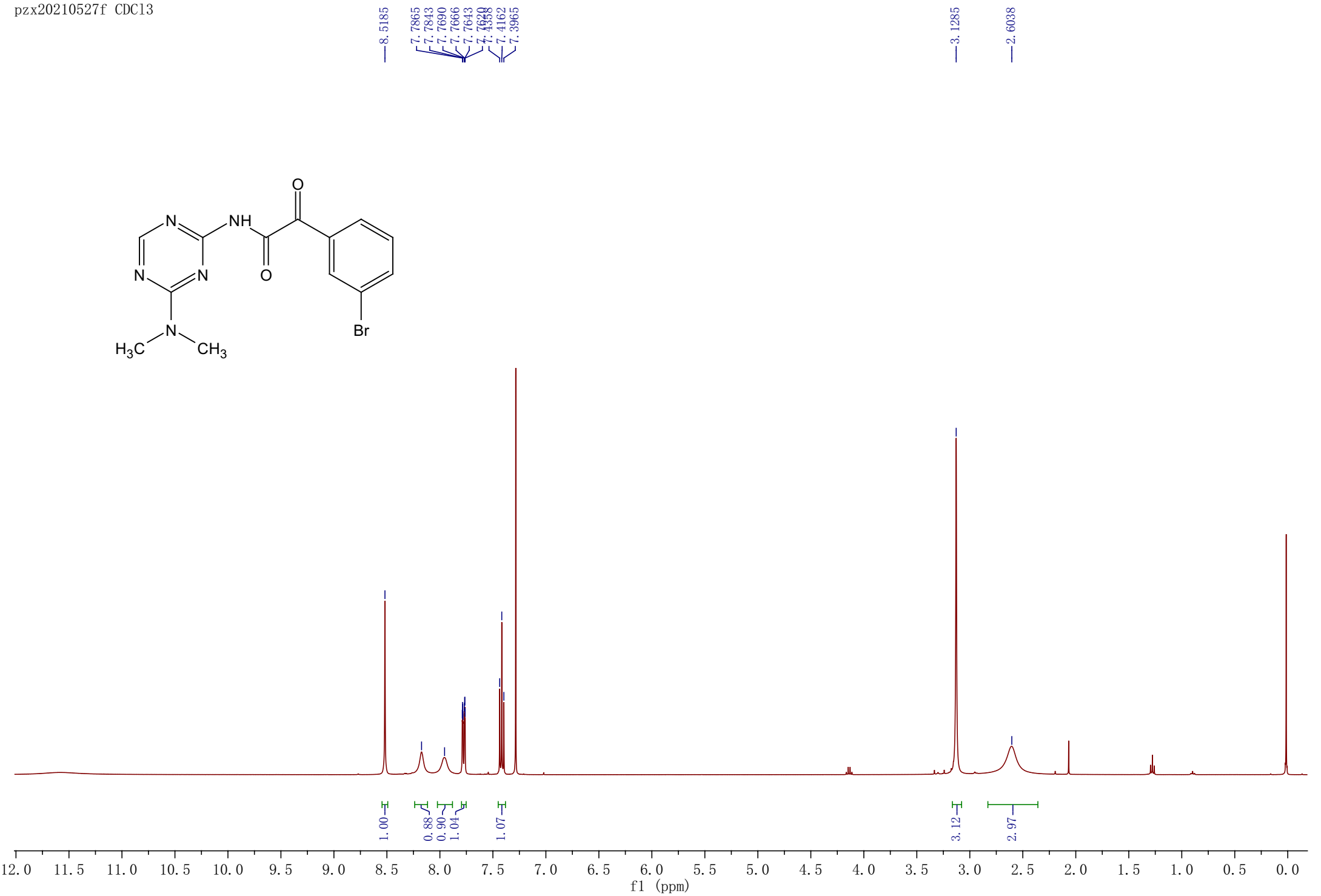
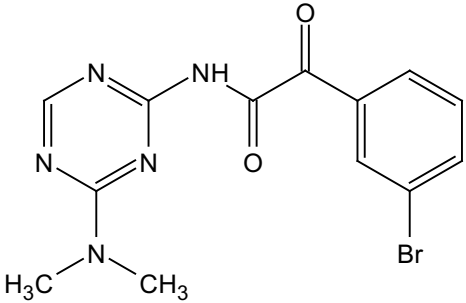






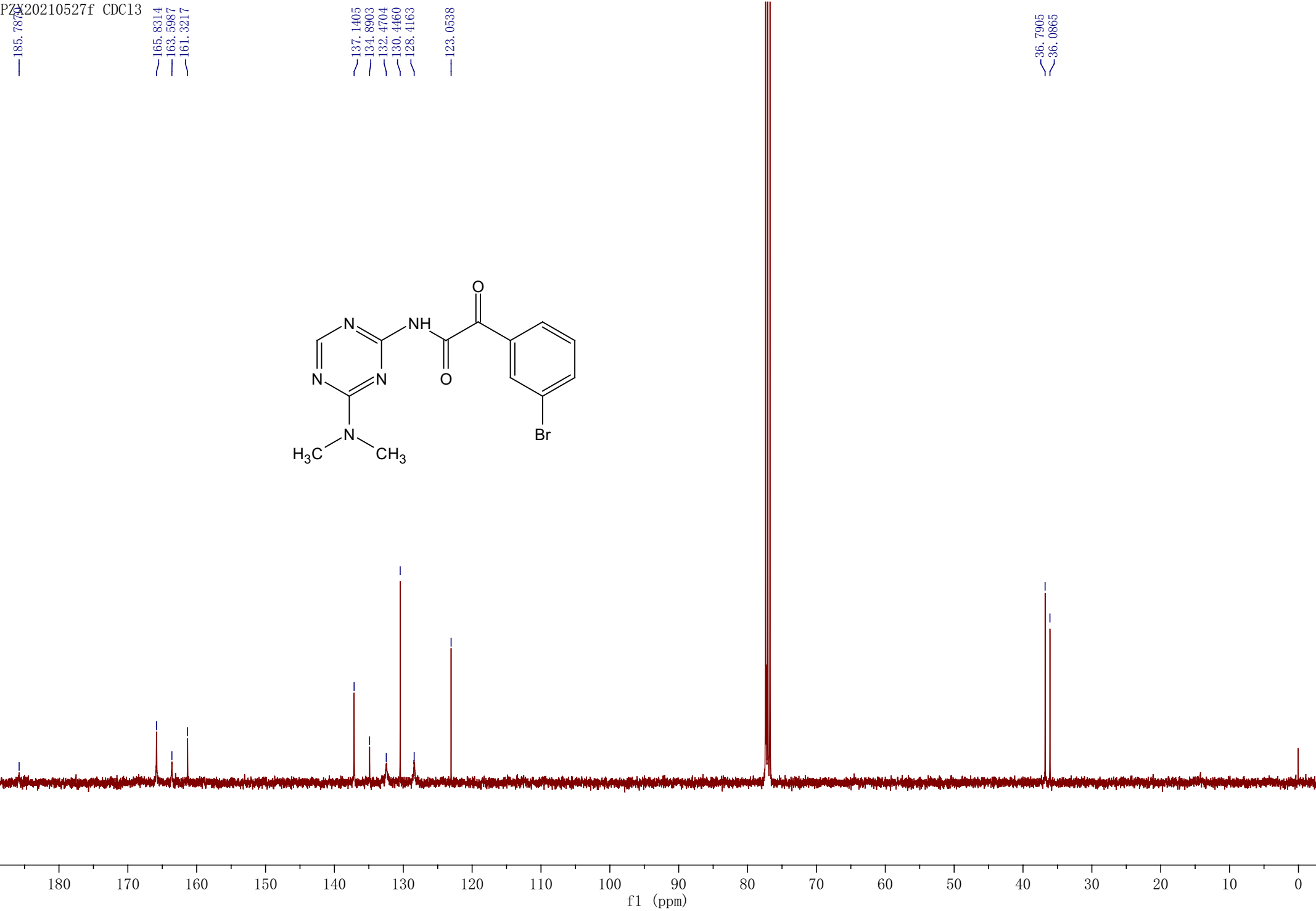
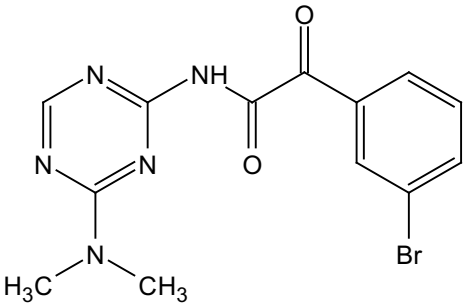
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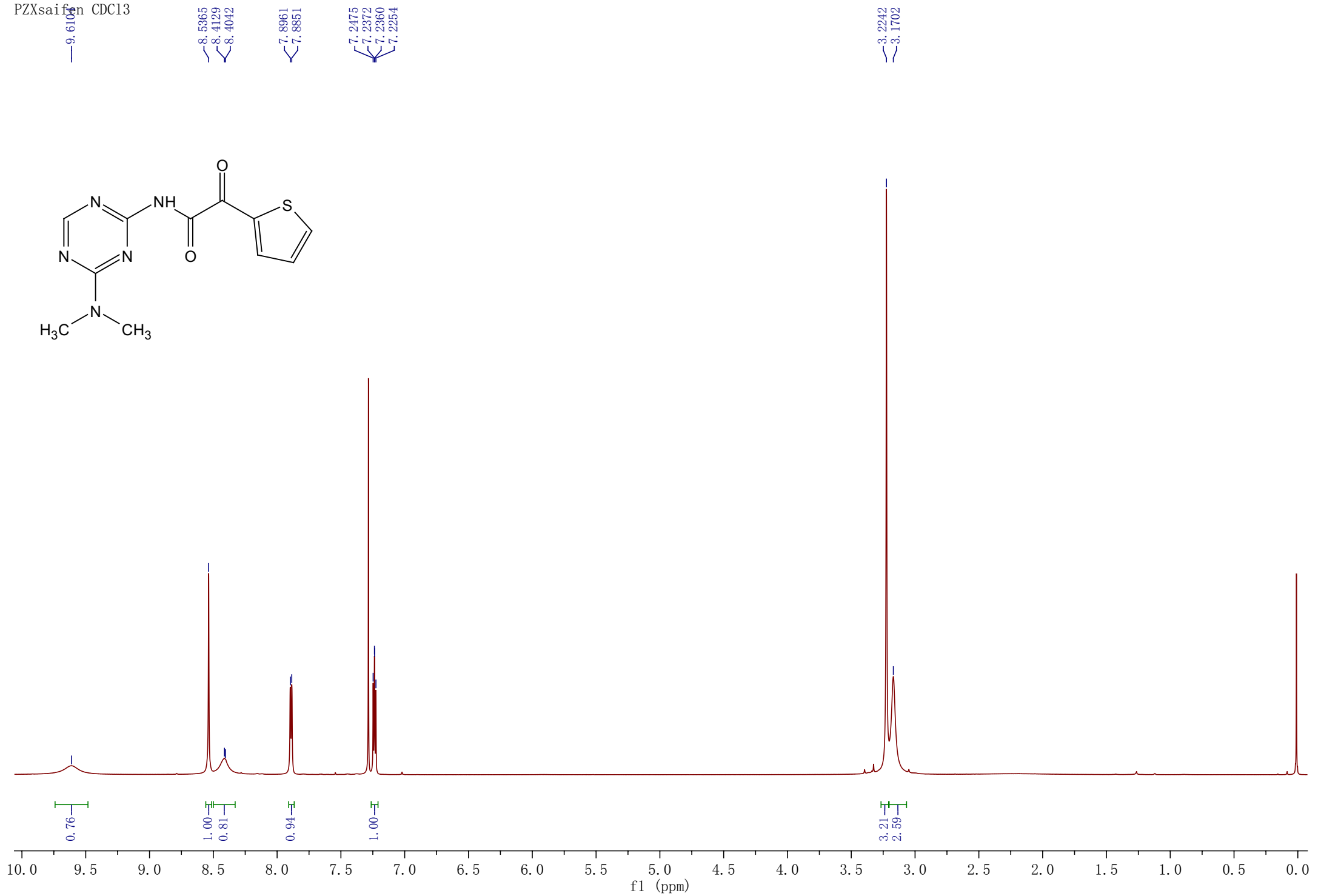
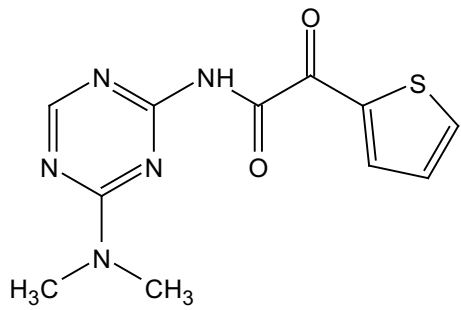


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PZXsaifen CDC13



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P2XSAIFEN

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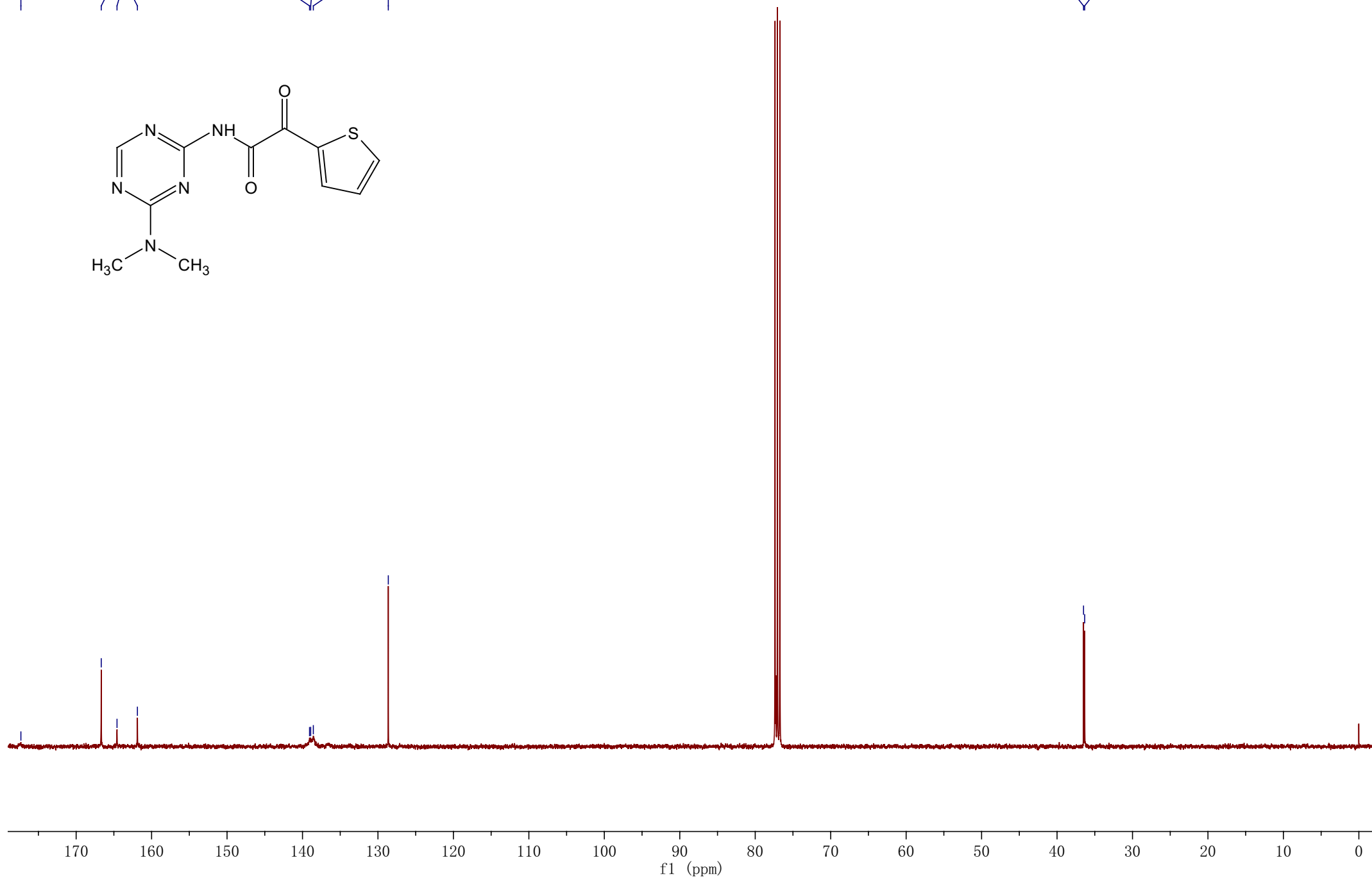
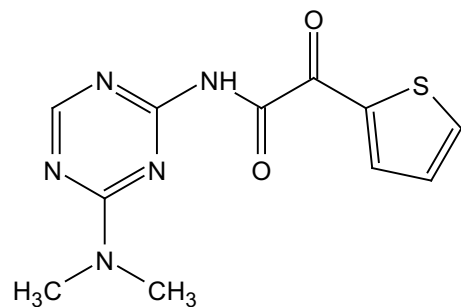
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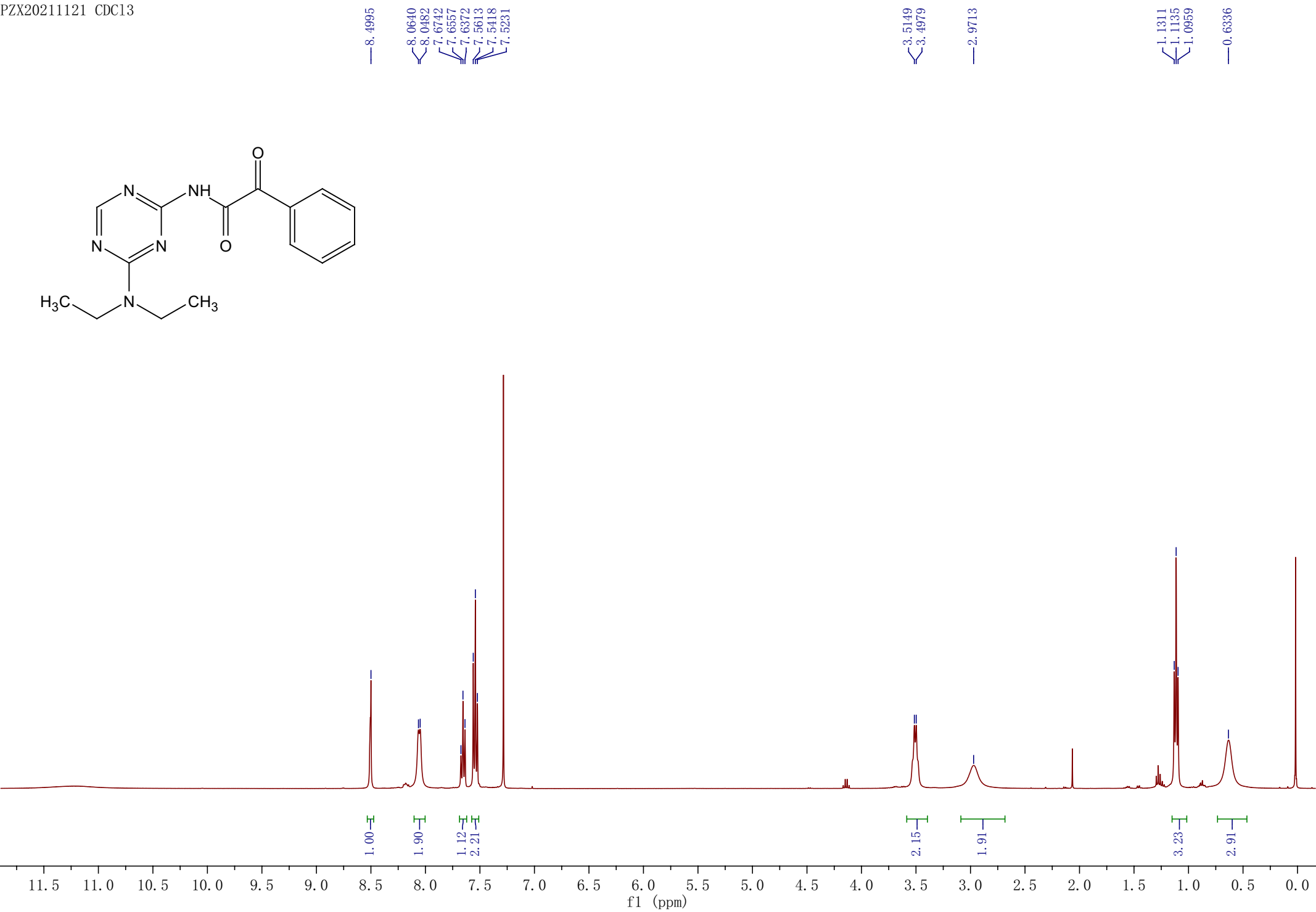
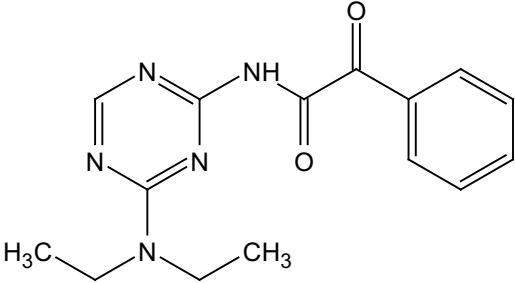
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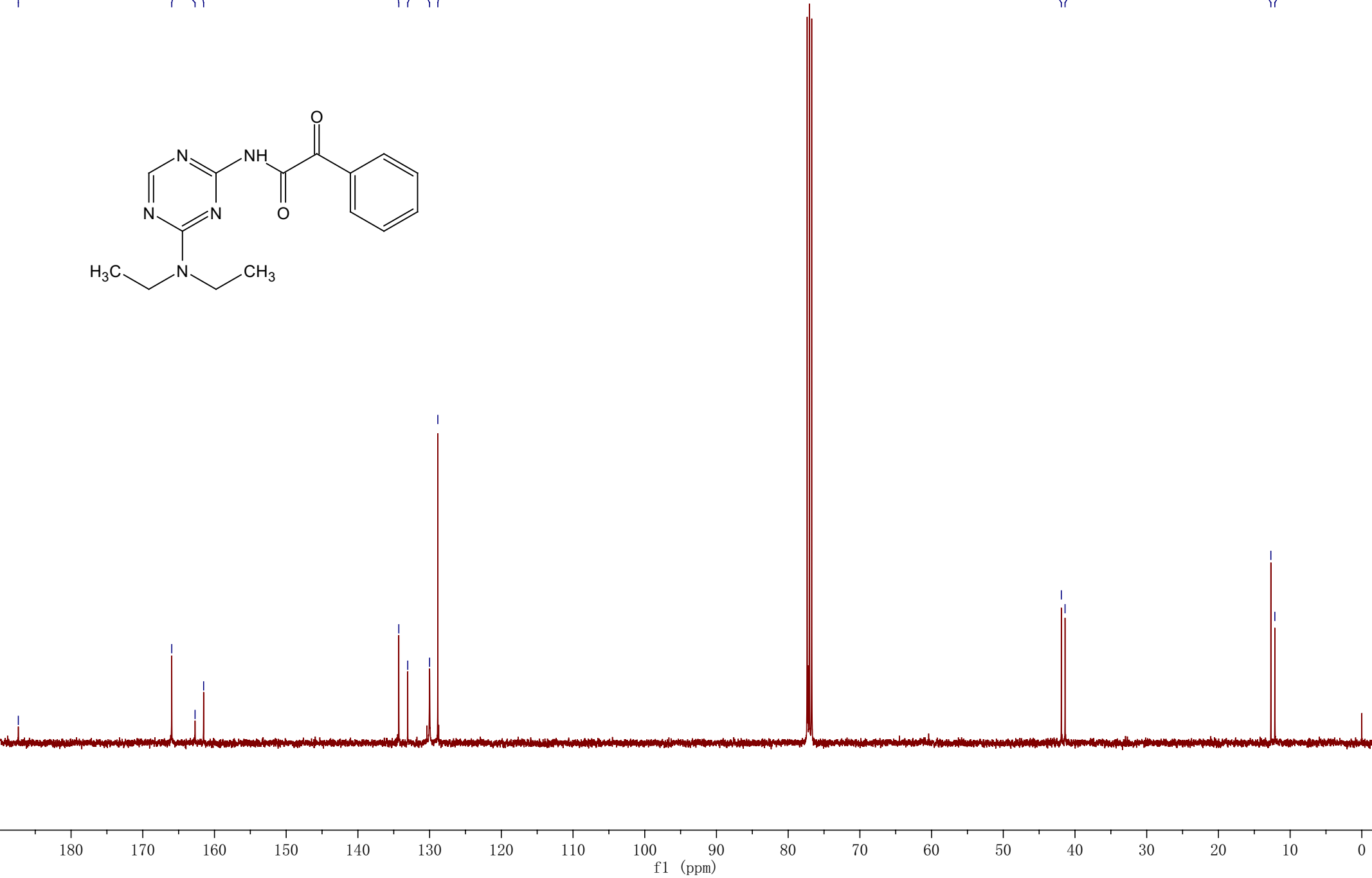
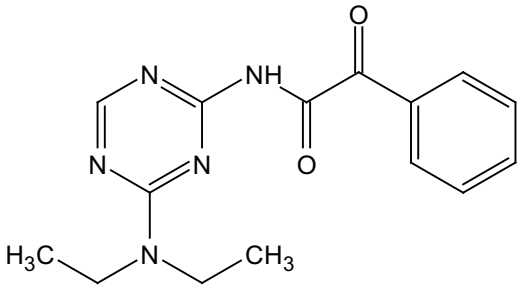
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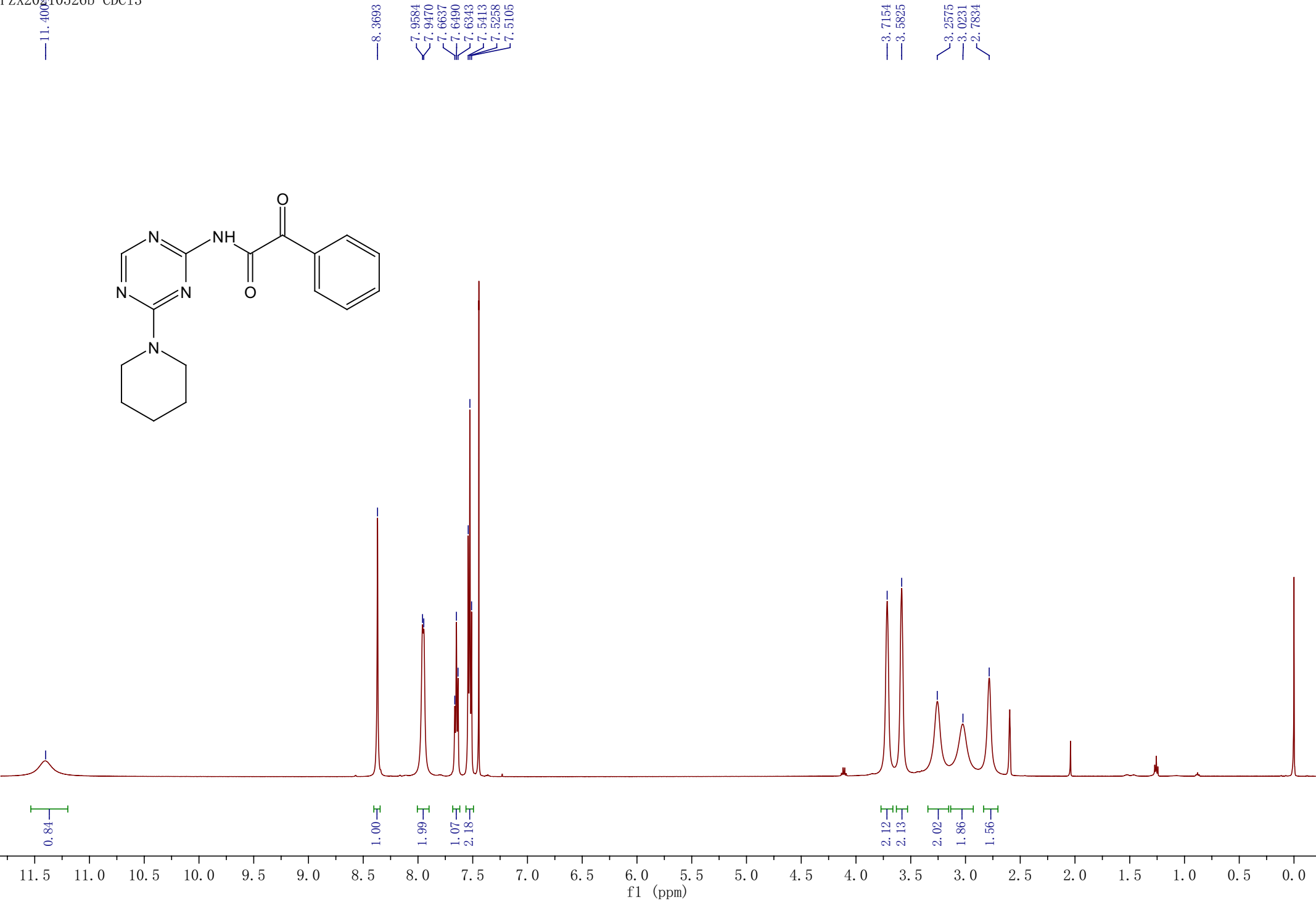
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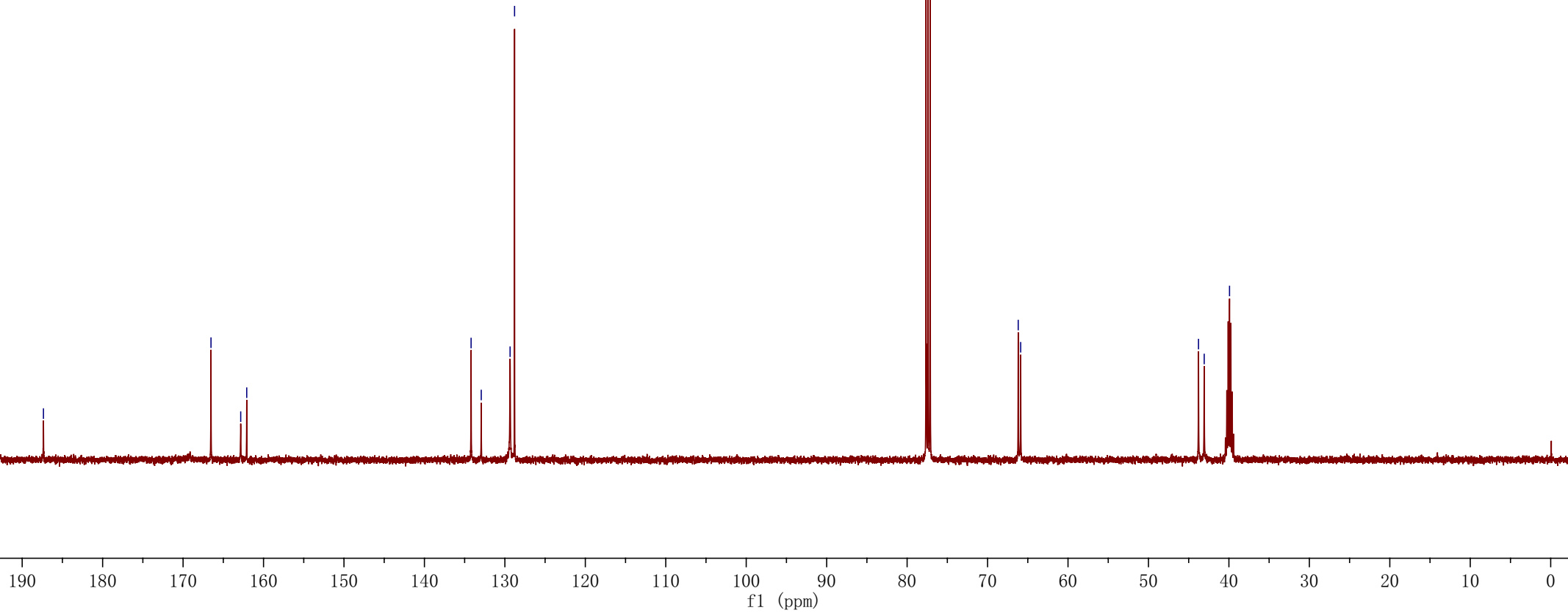
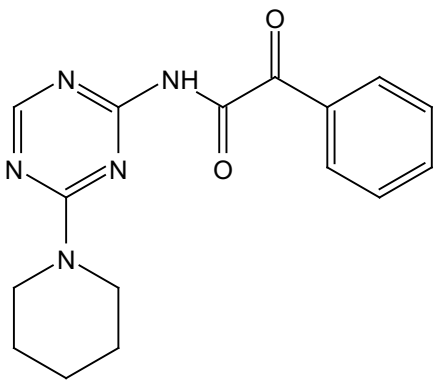
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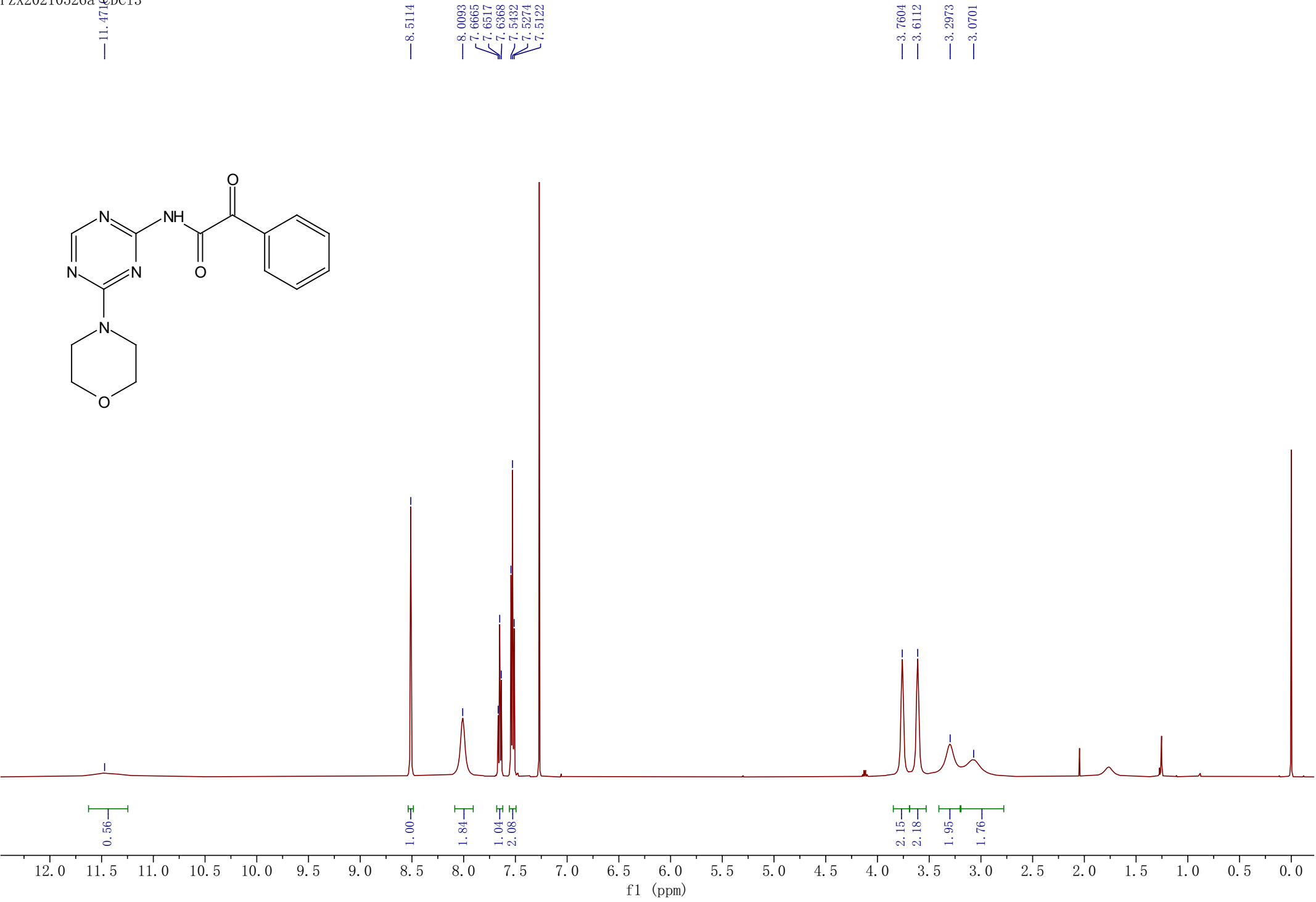
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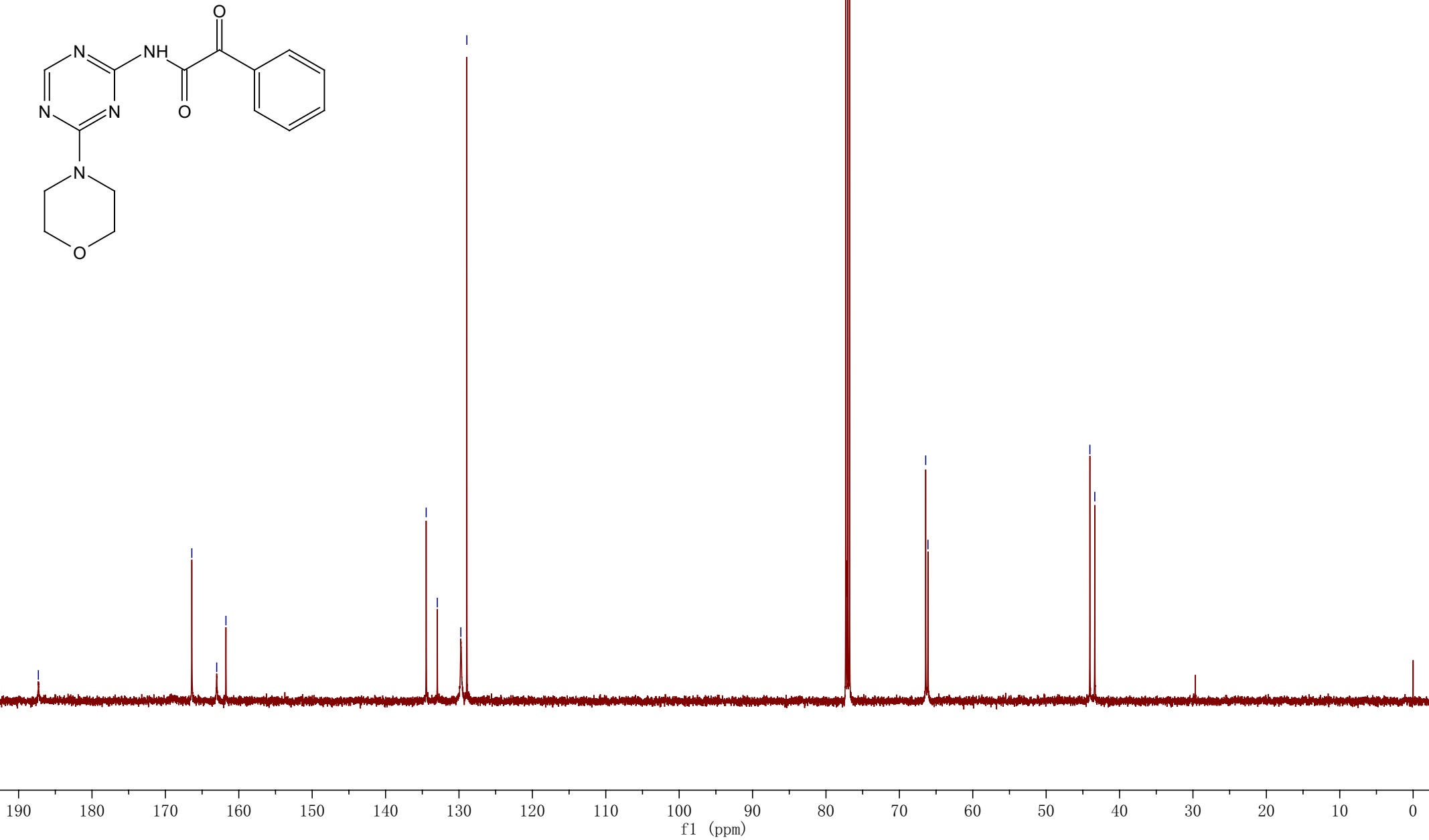


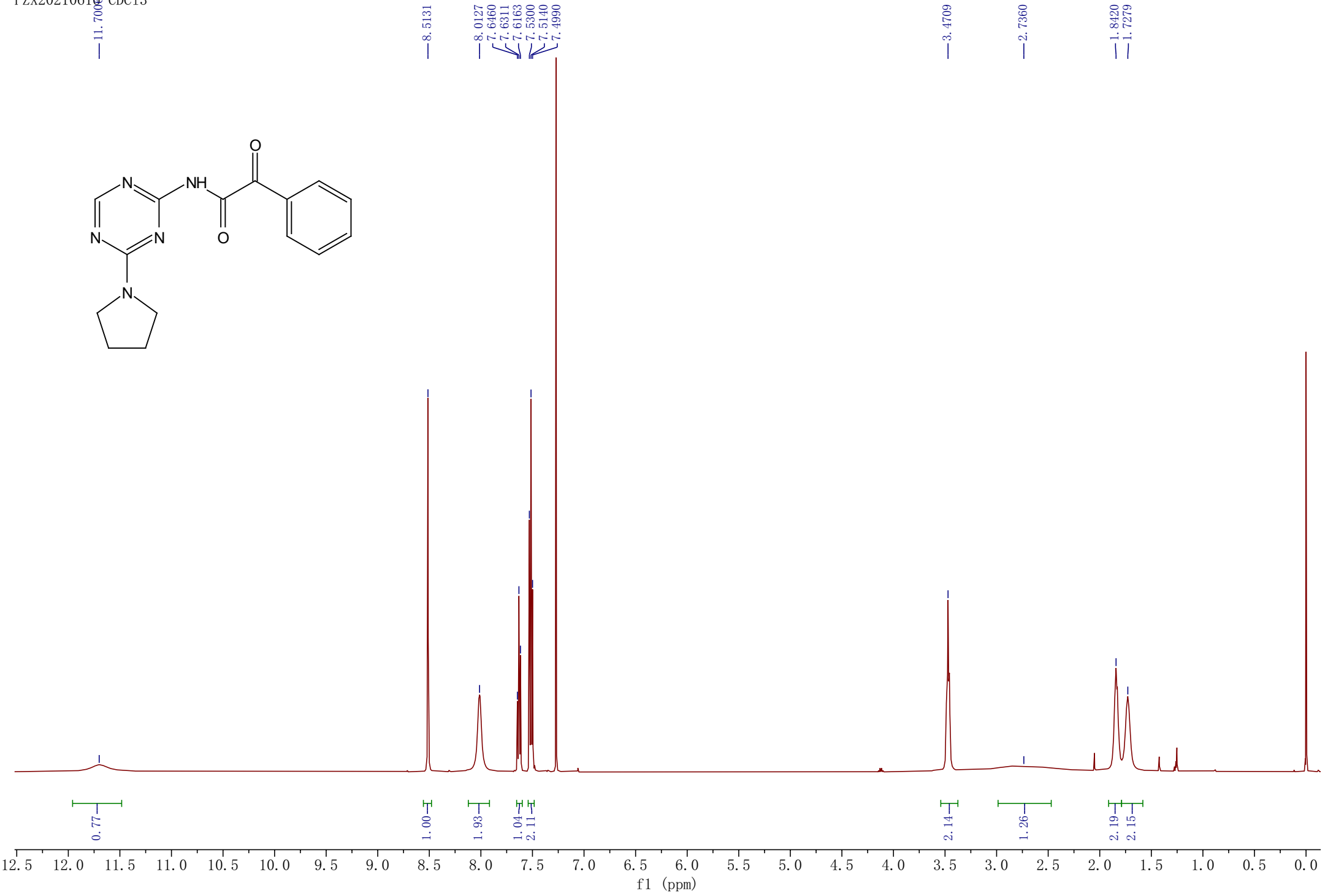
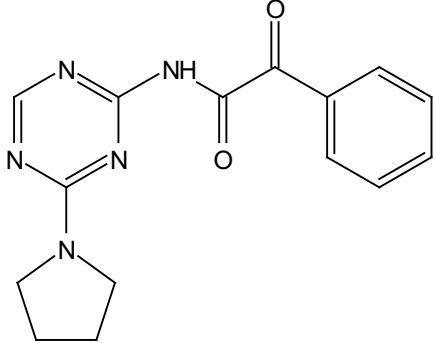


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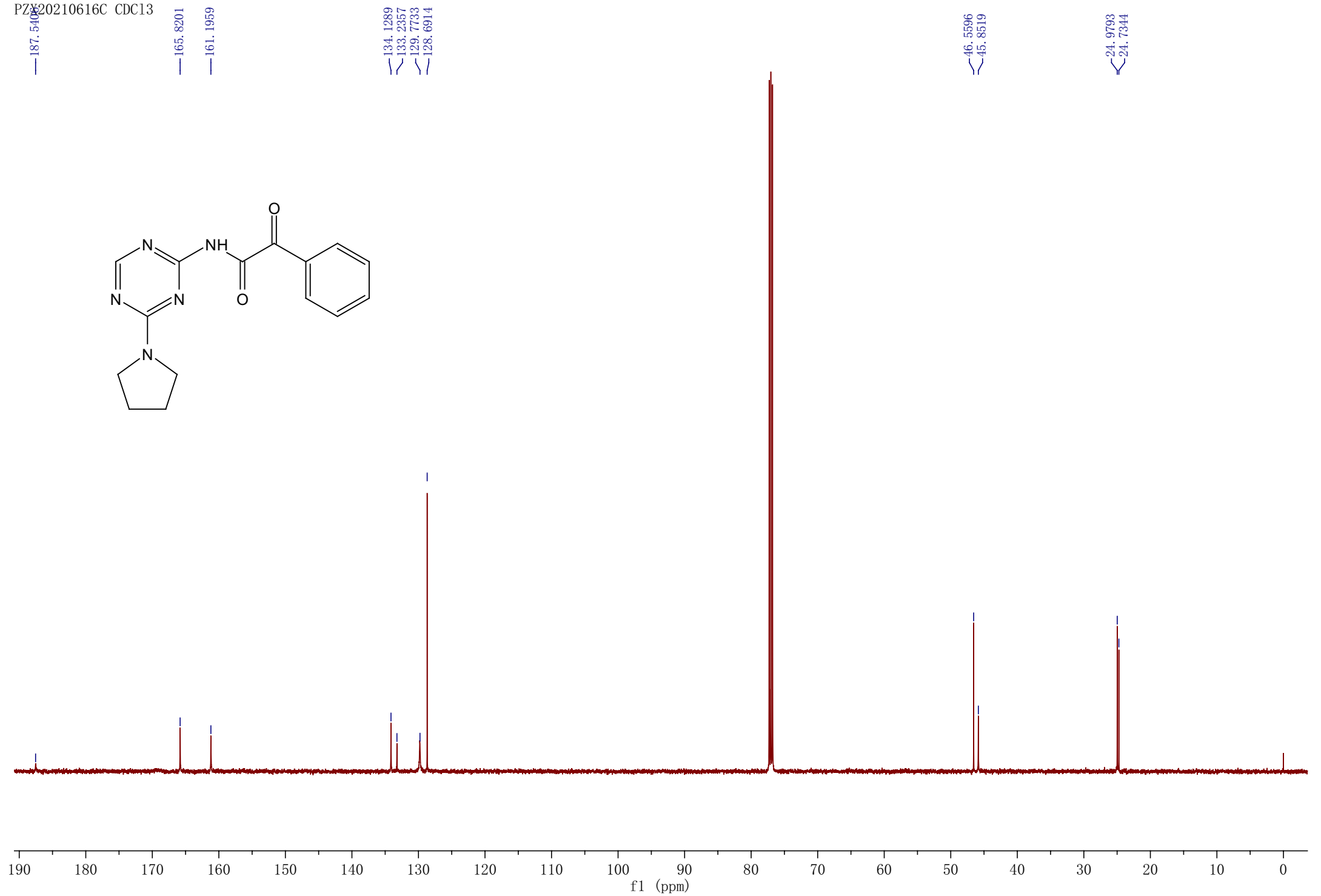
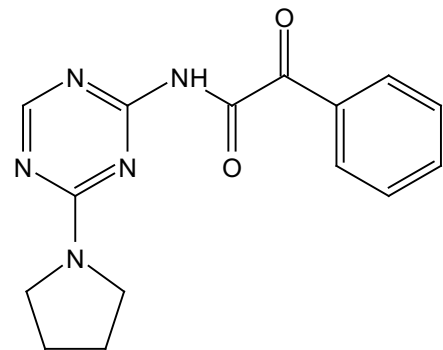


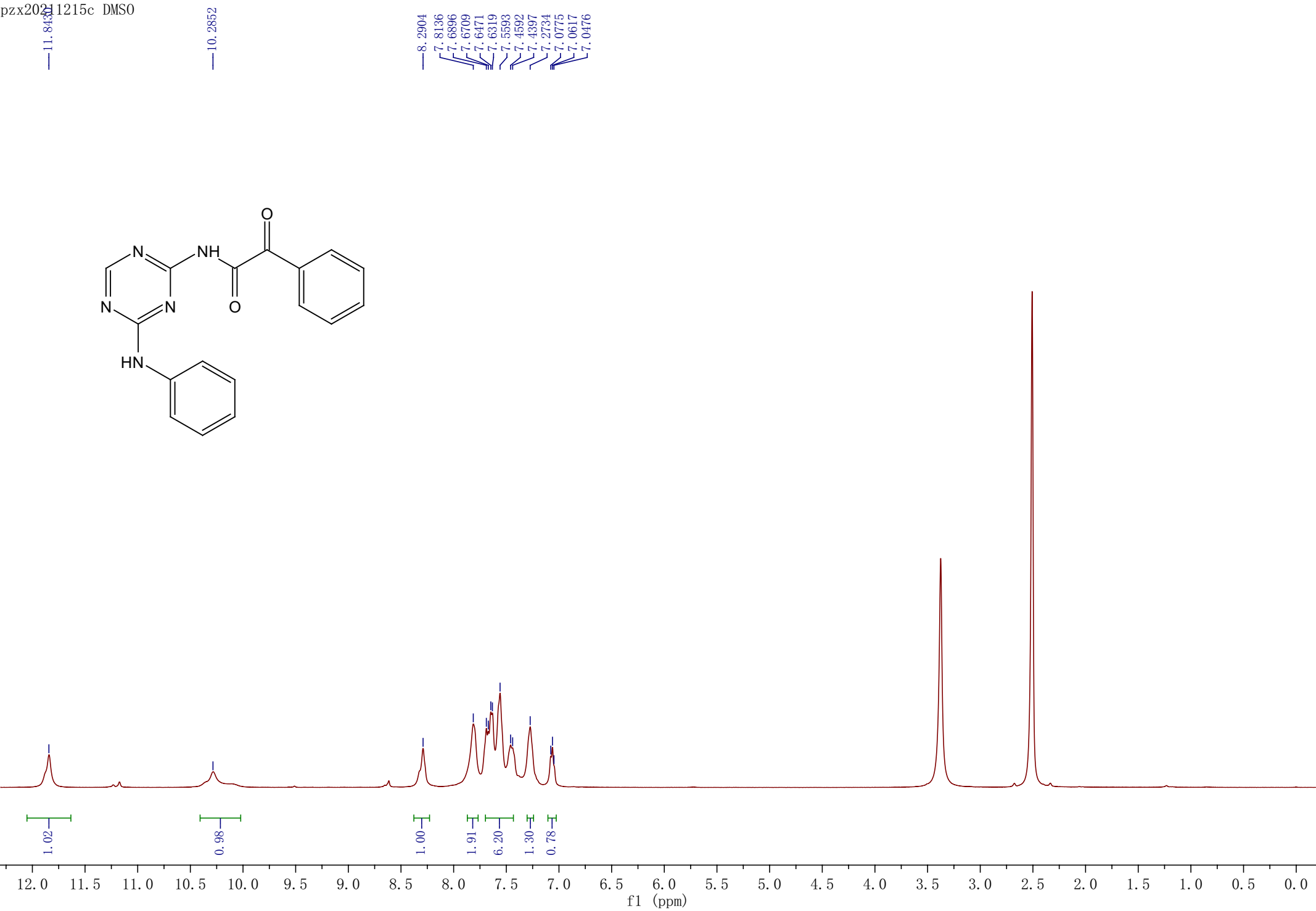




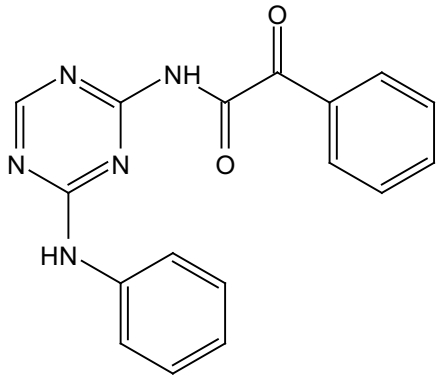


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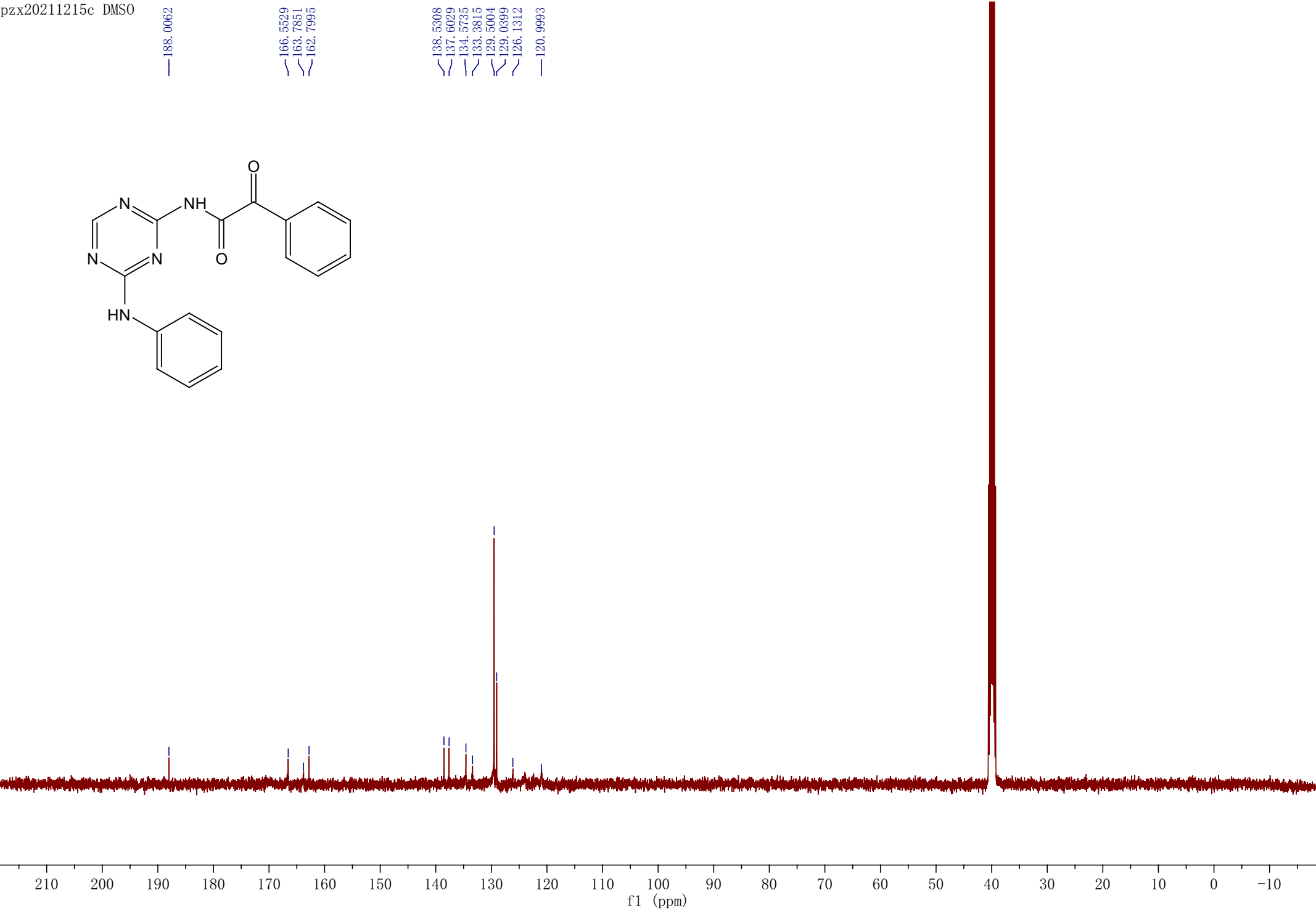




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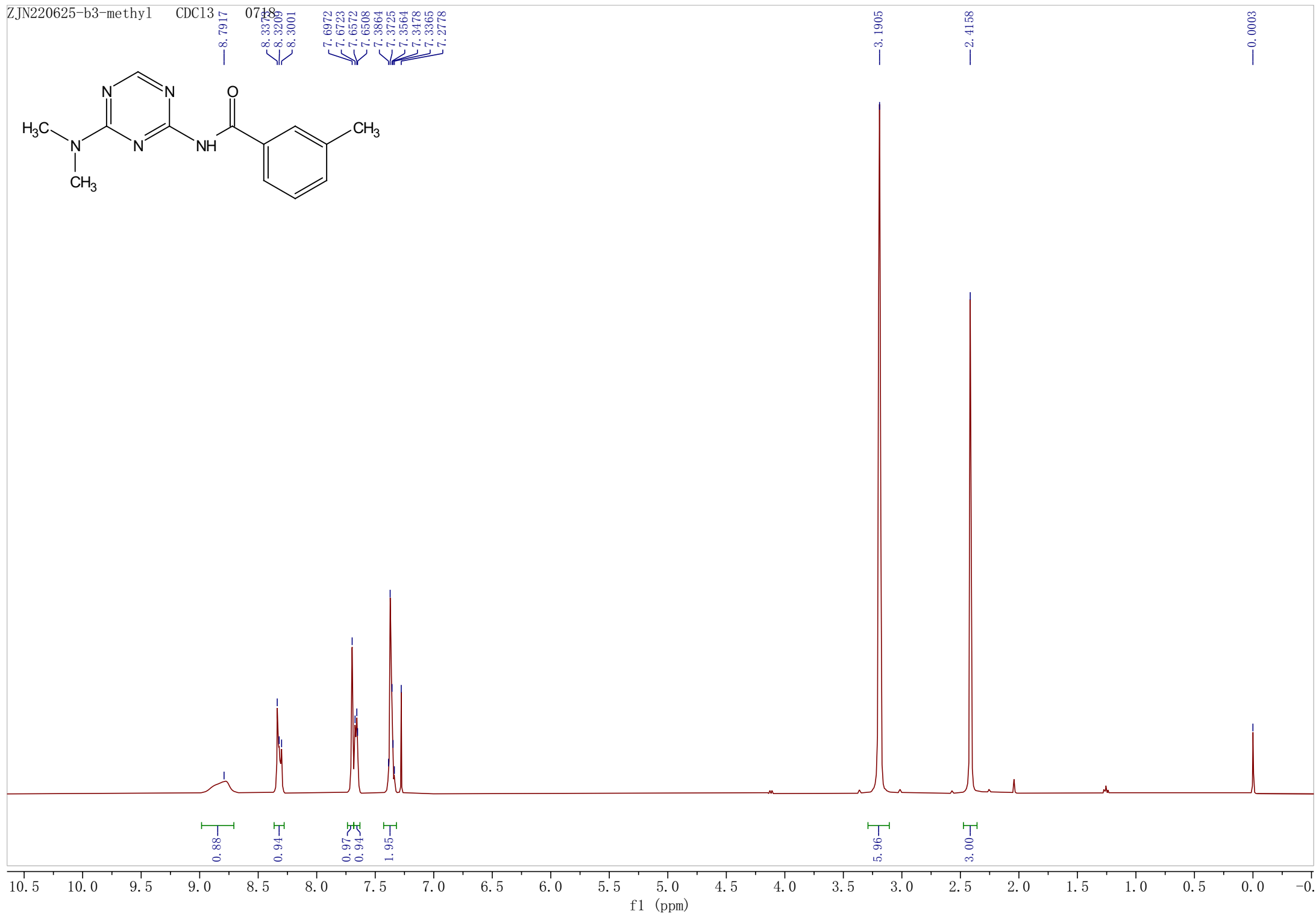
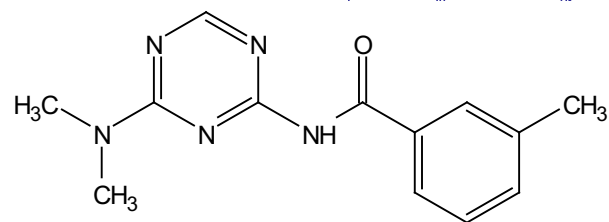
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ZJN220625-b3-methyl

CDC13

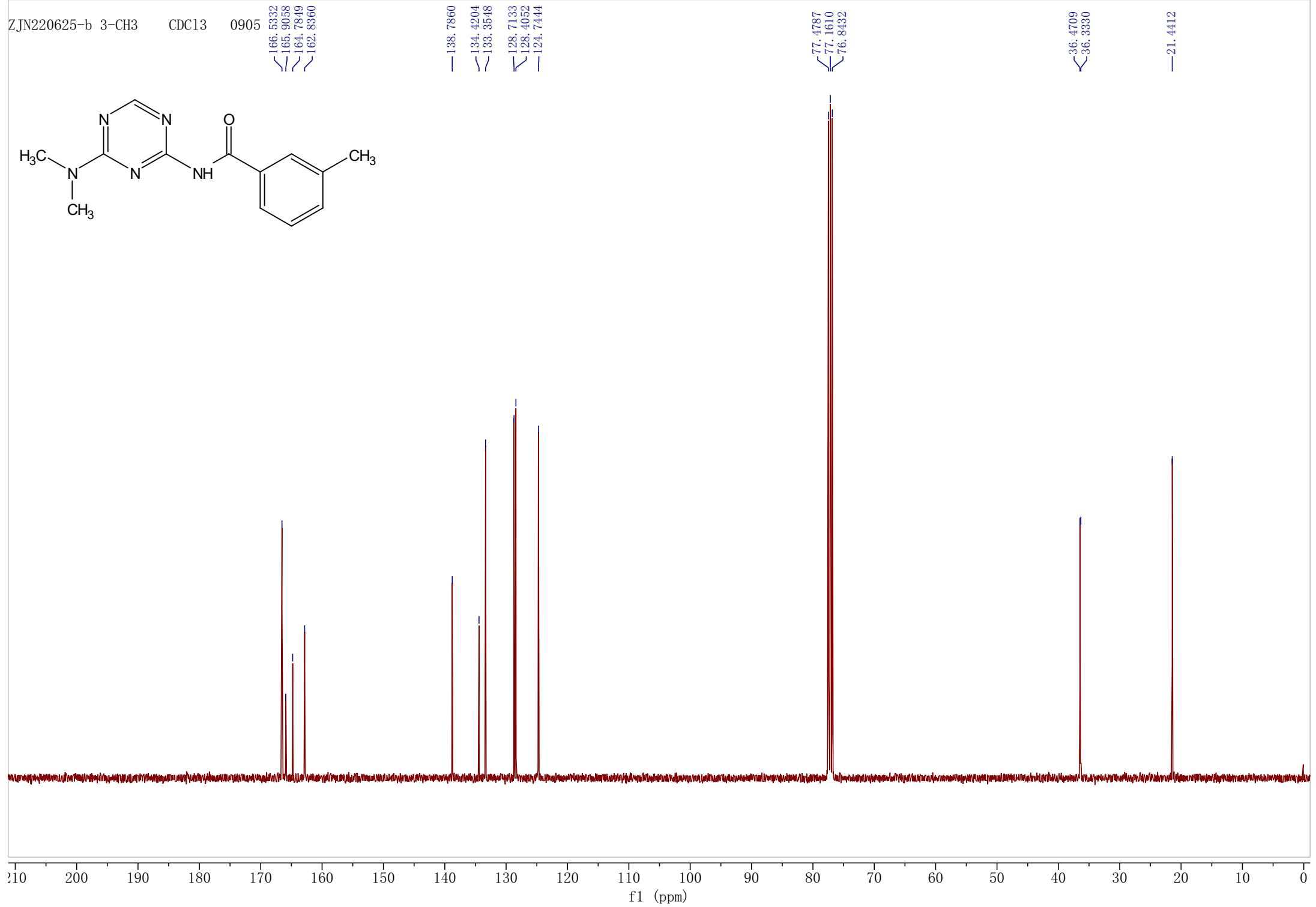
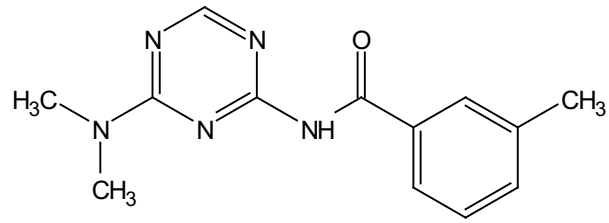
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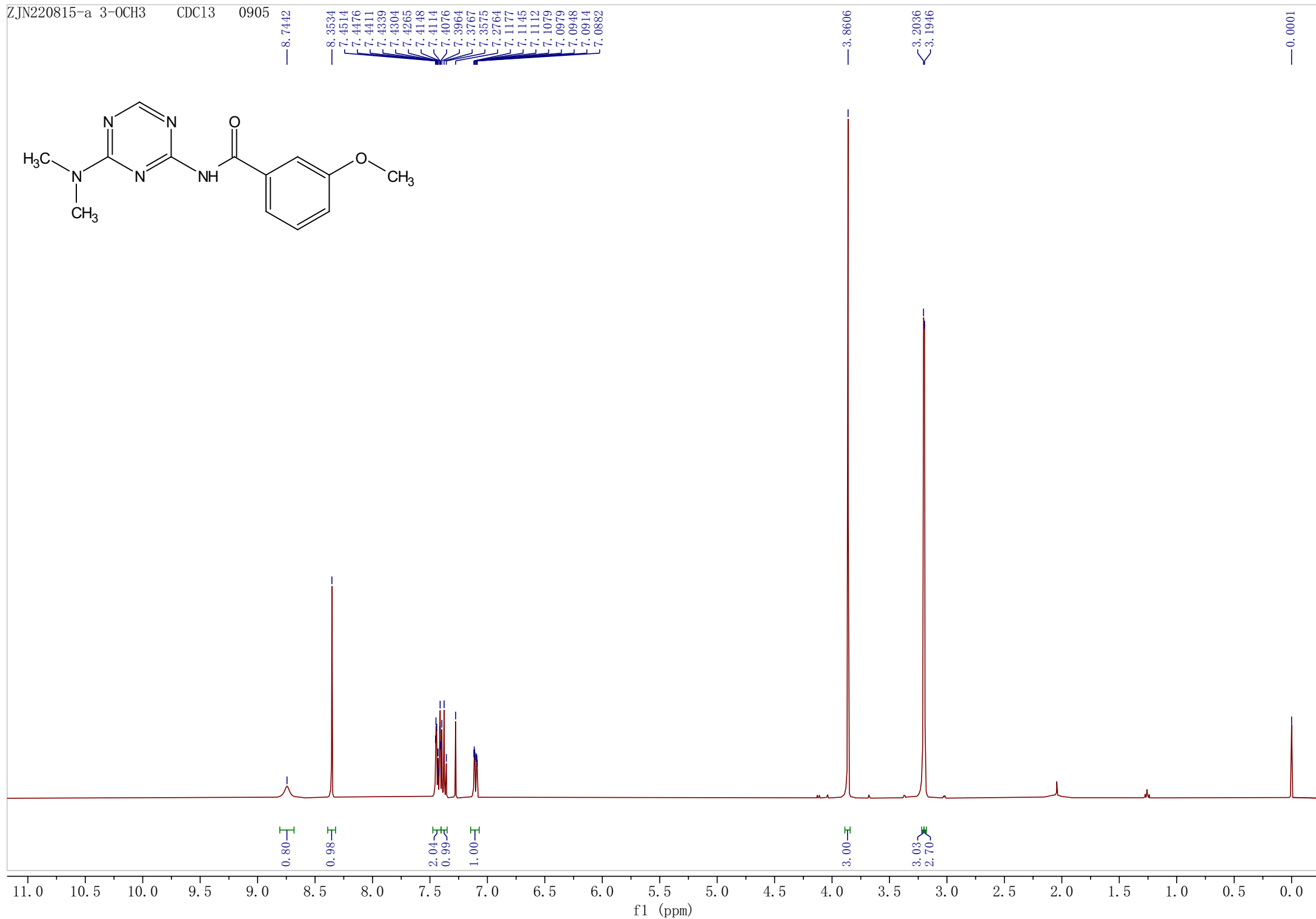
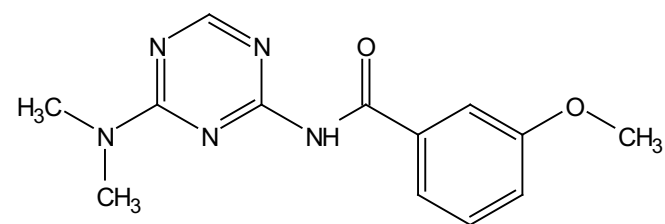


ZJN220625-b 3-CH3

CDC13

0905





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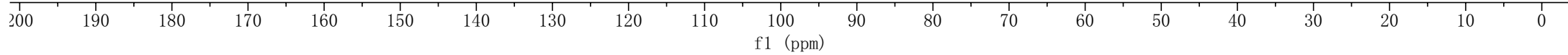
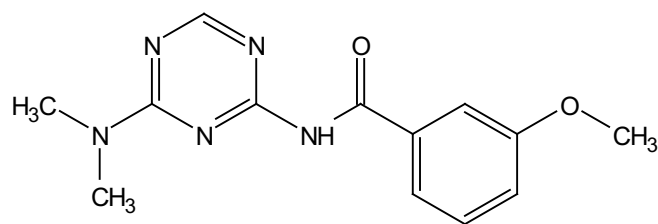
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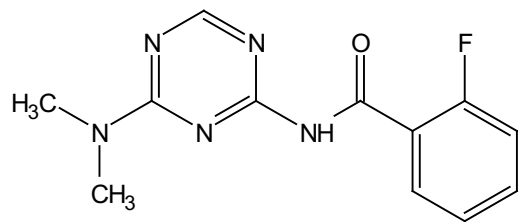
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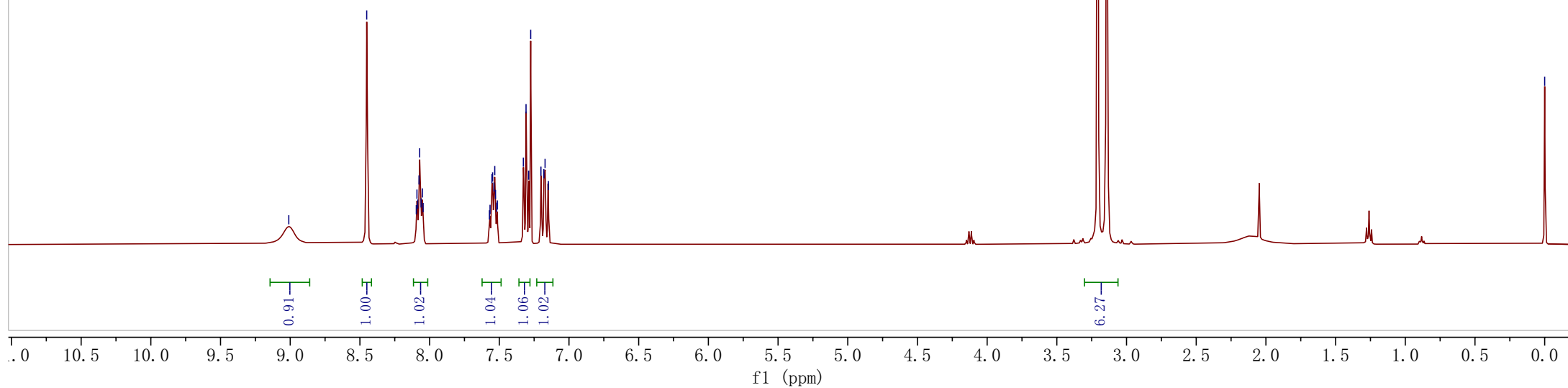
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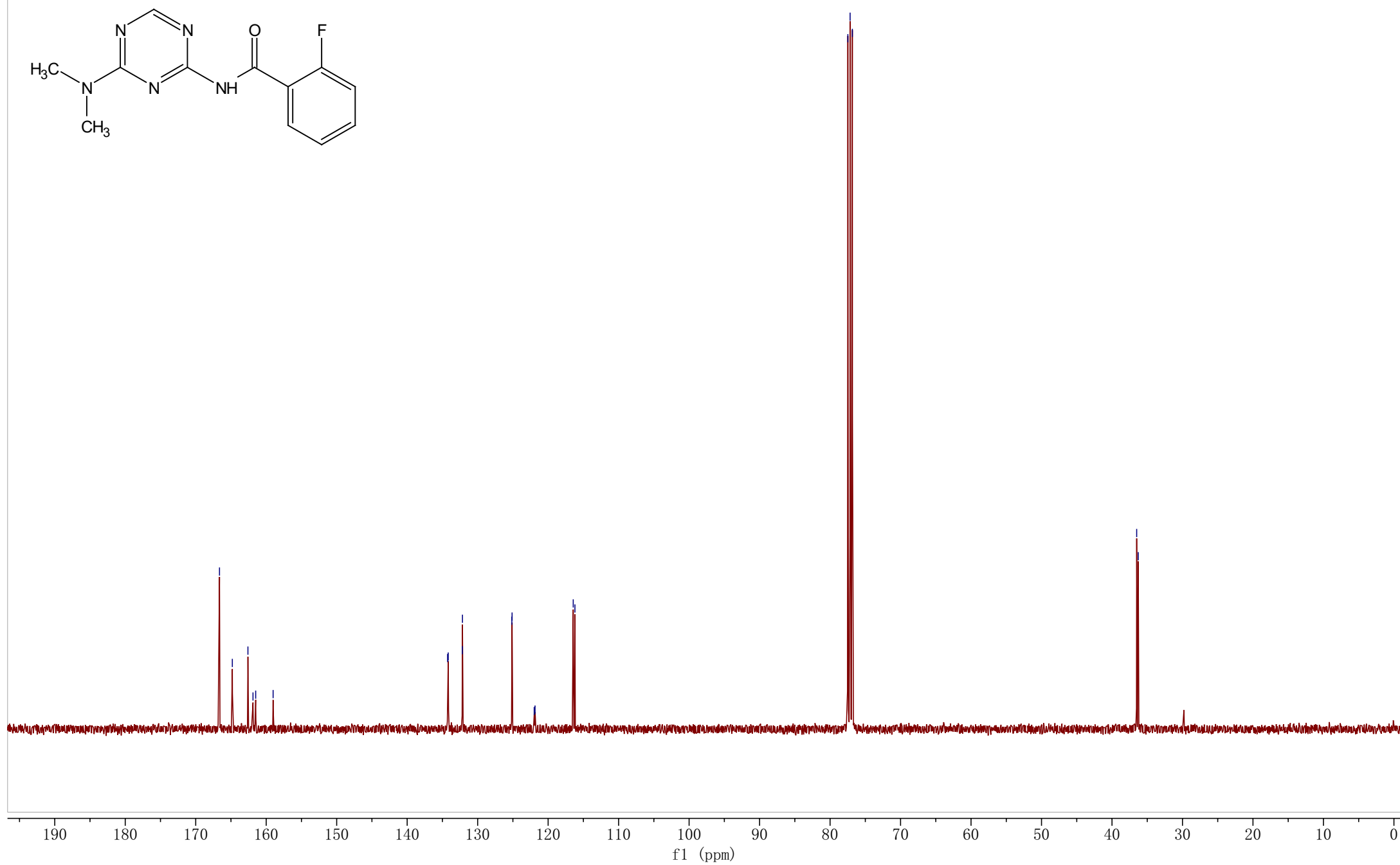
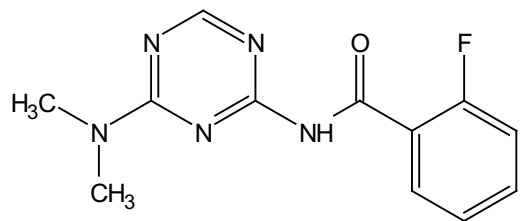
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CDC13

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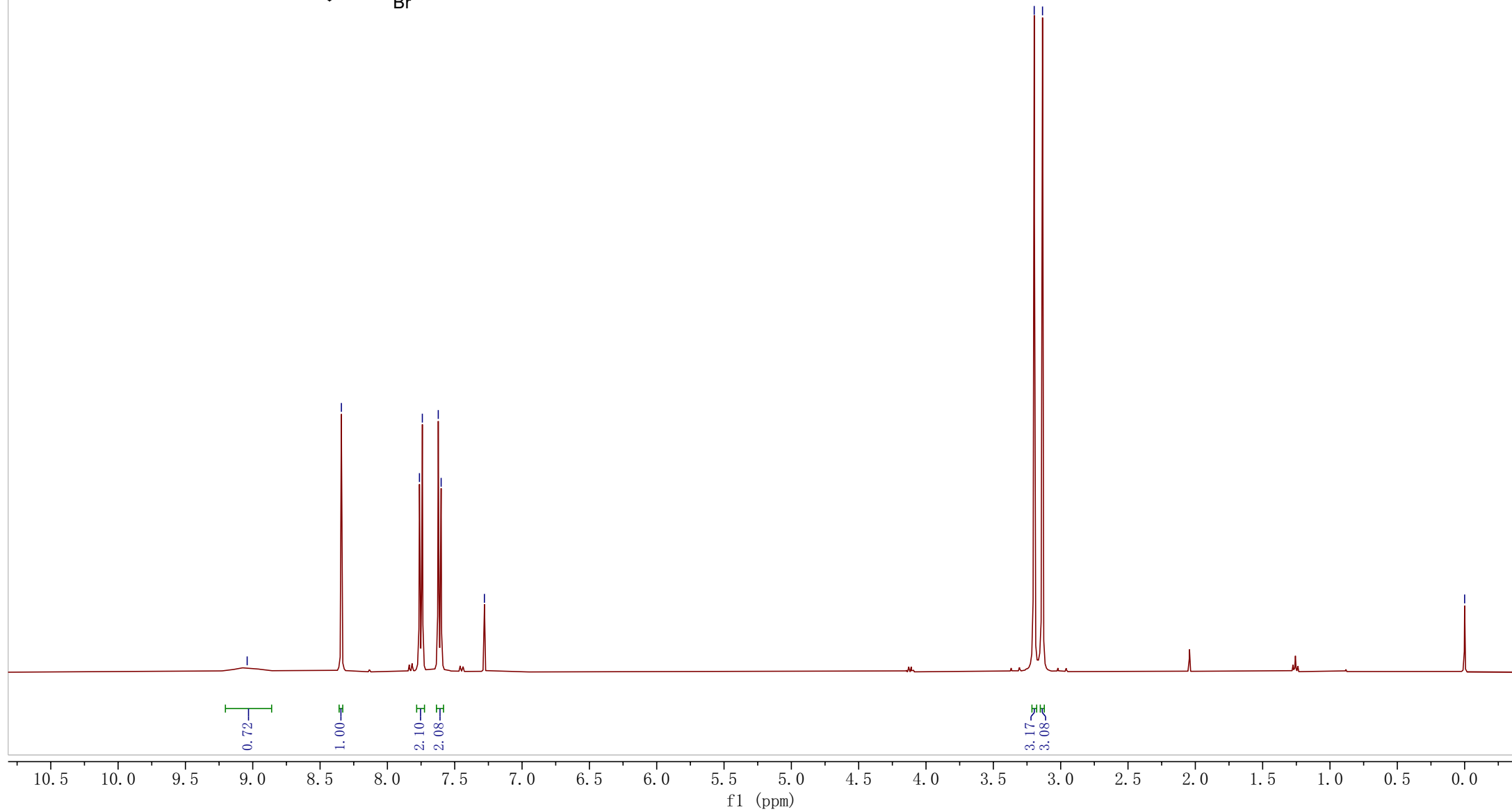
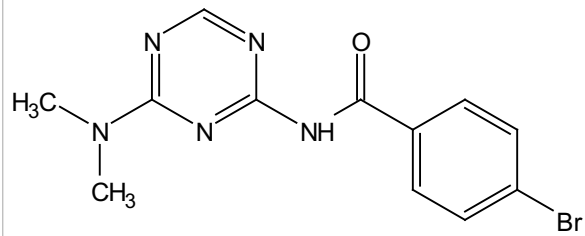
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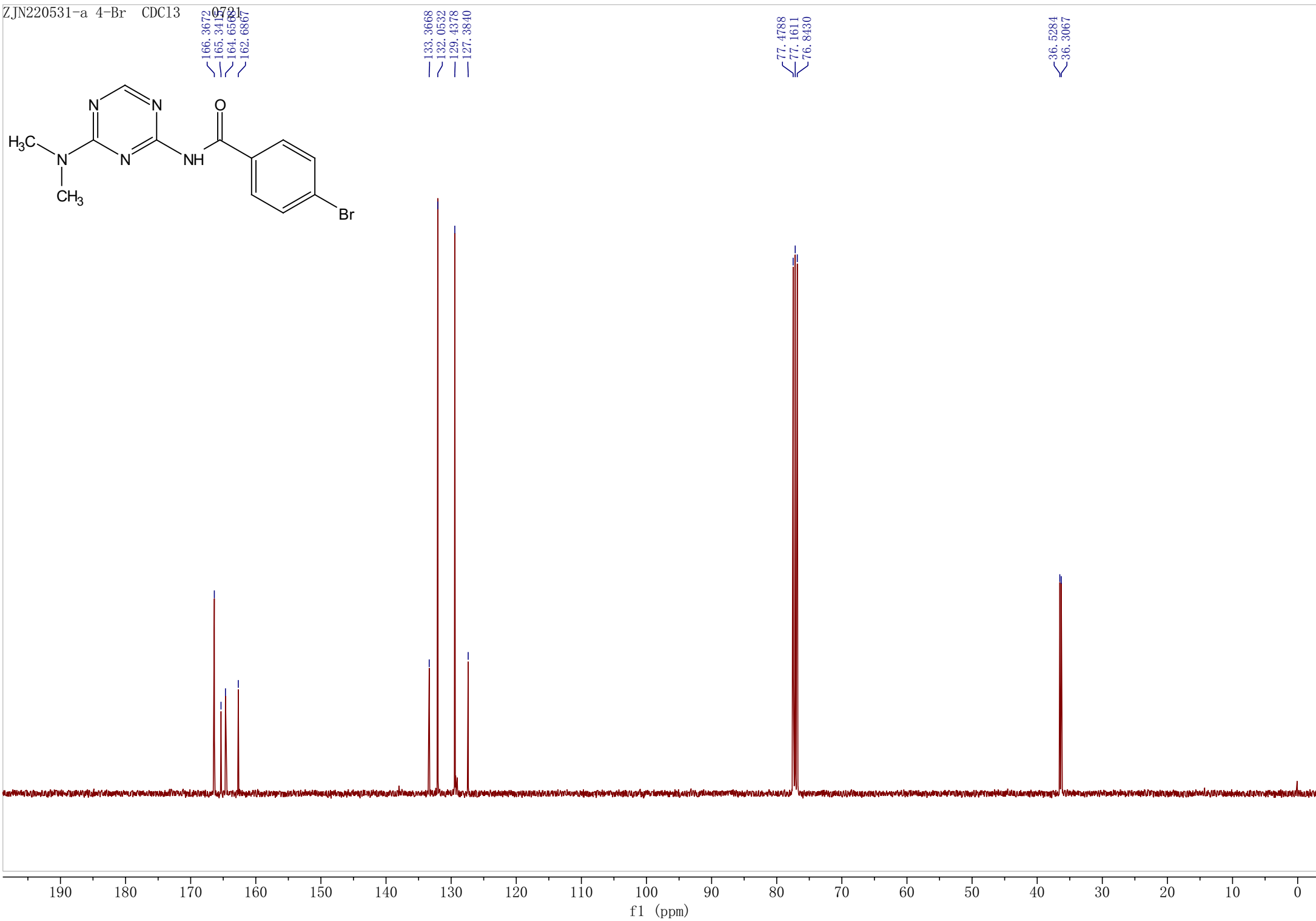
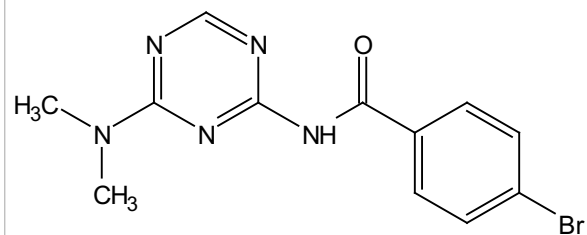
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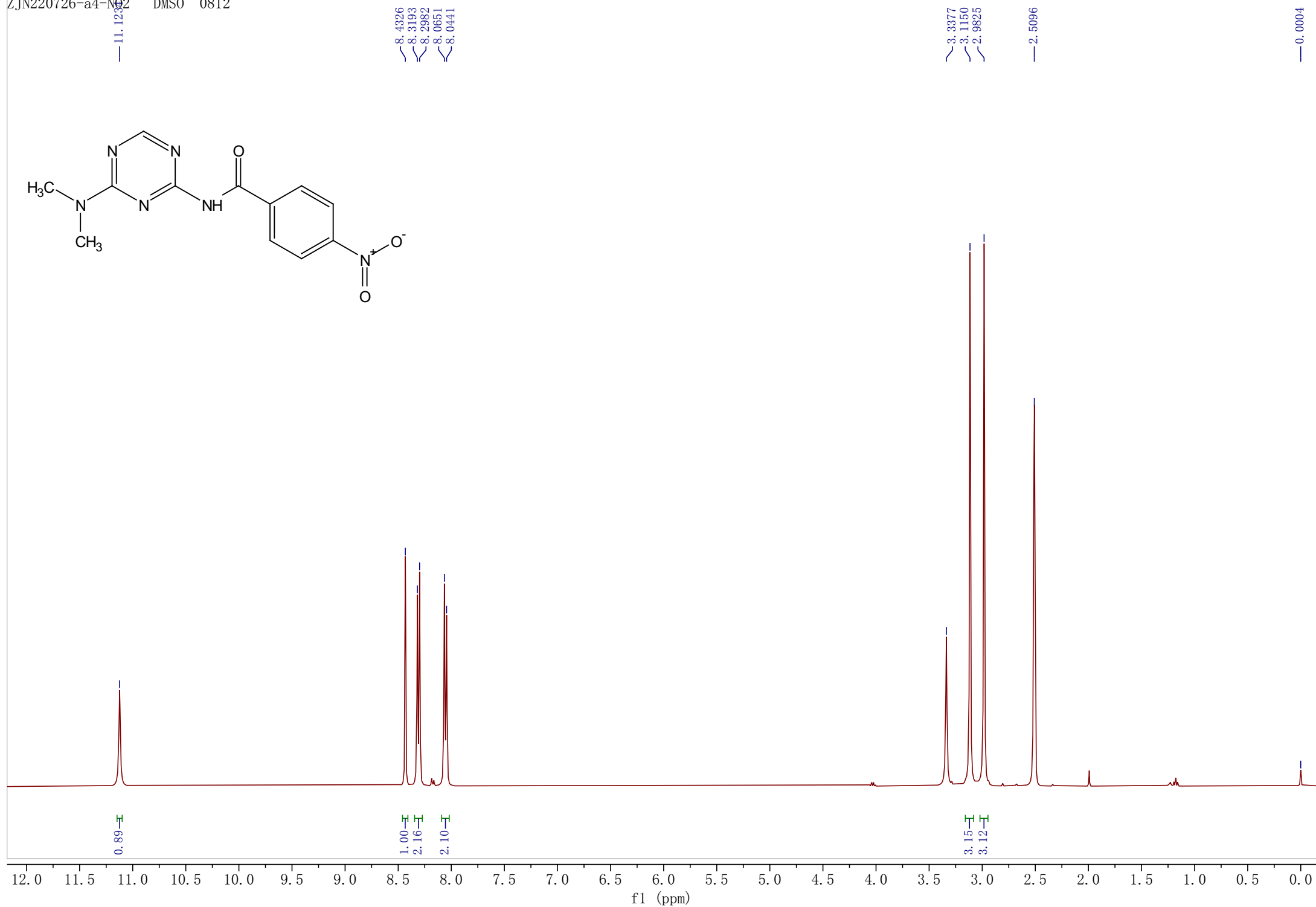
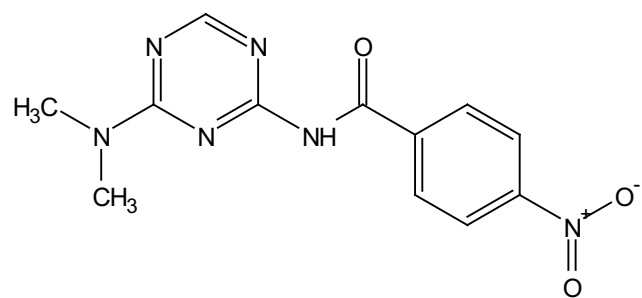
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-0.0000



ZJN220531-a 4-Br CDC13



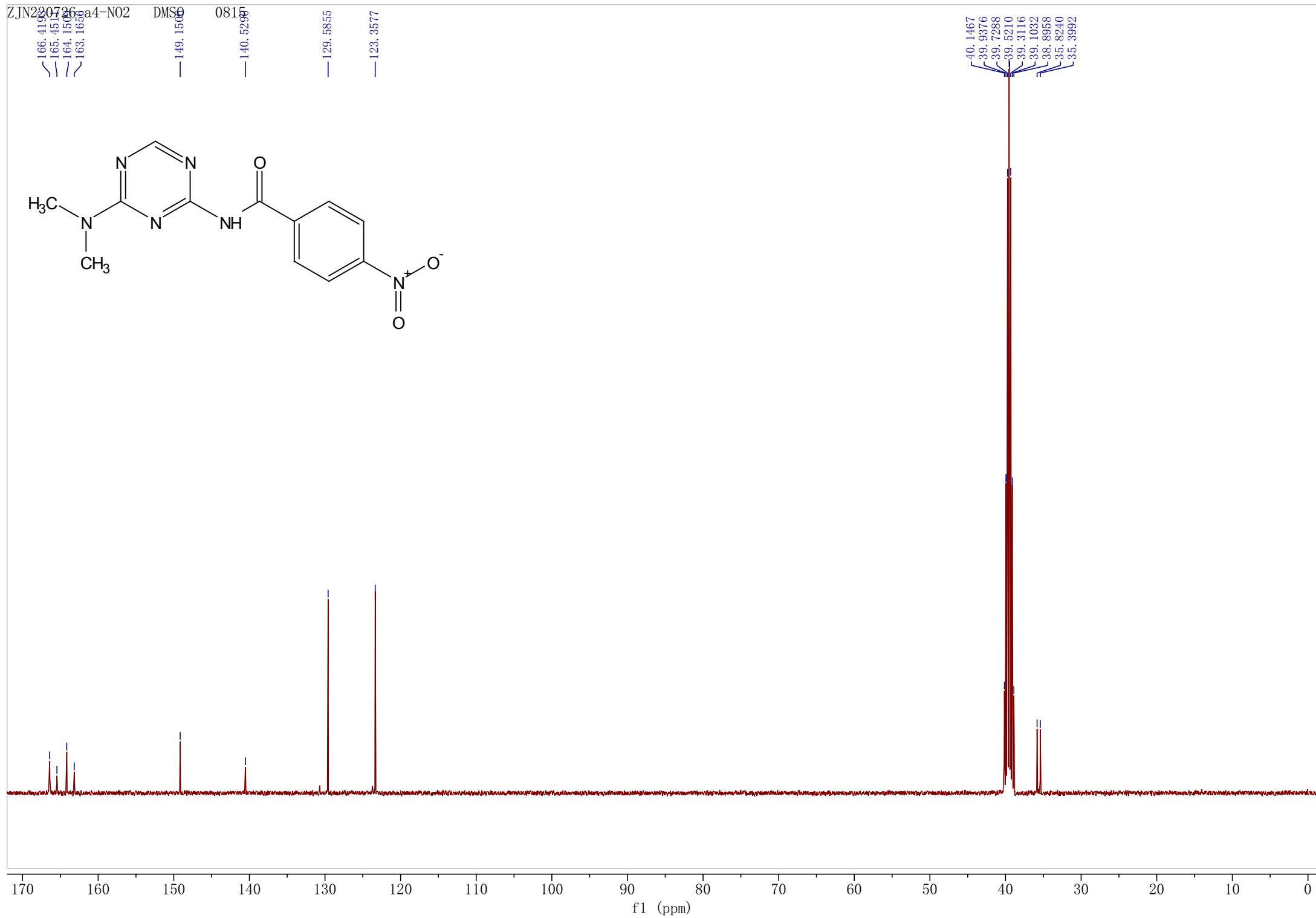
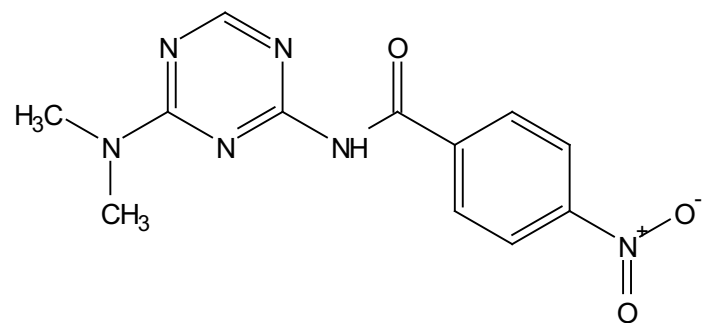


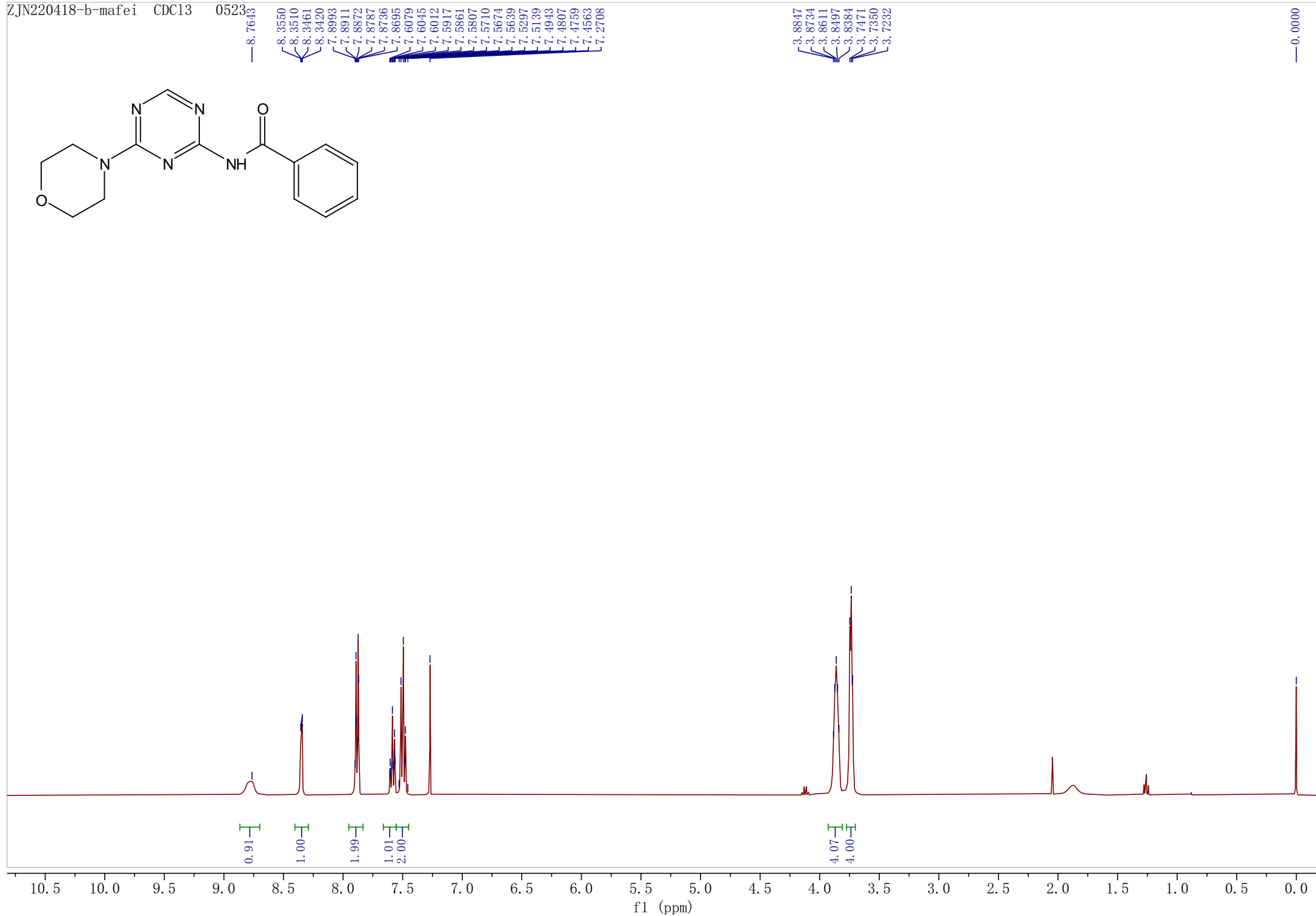
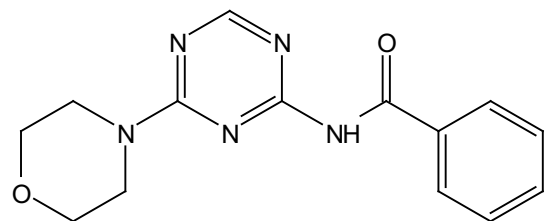
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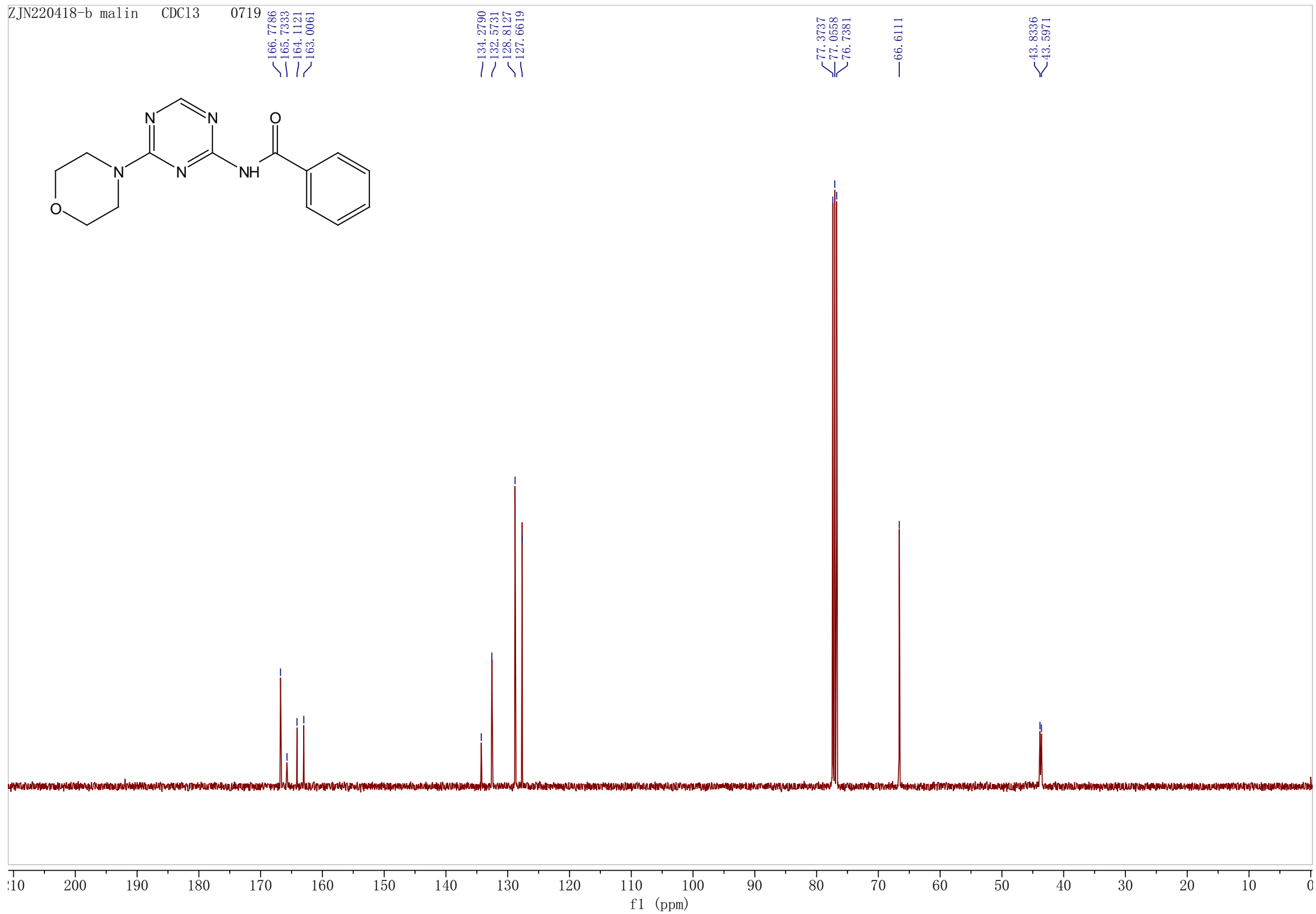
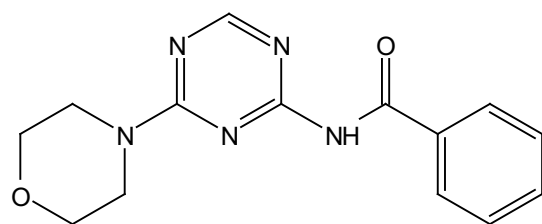
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0815

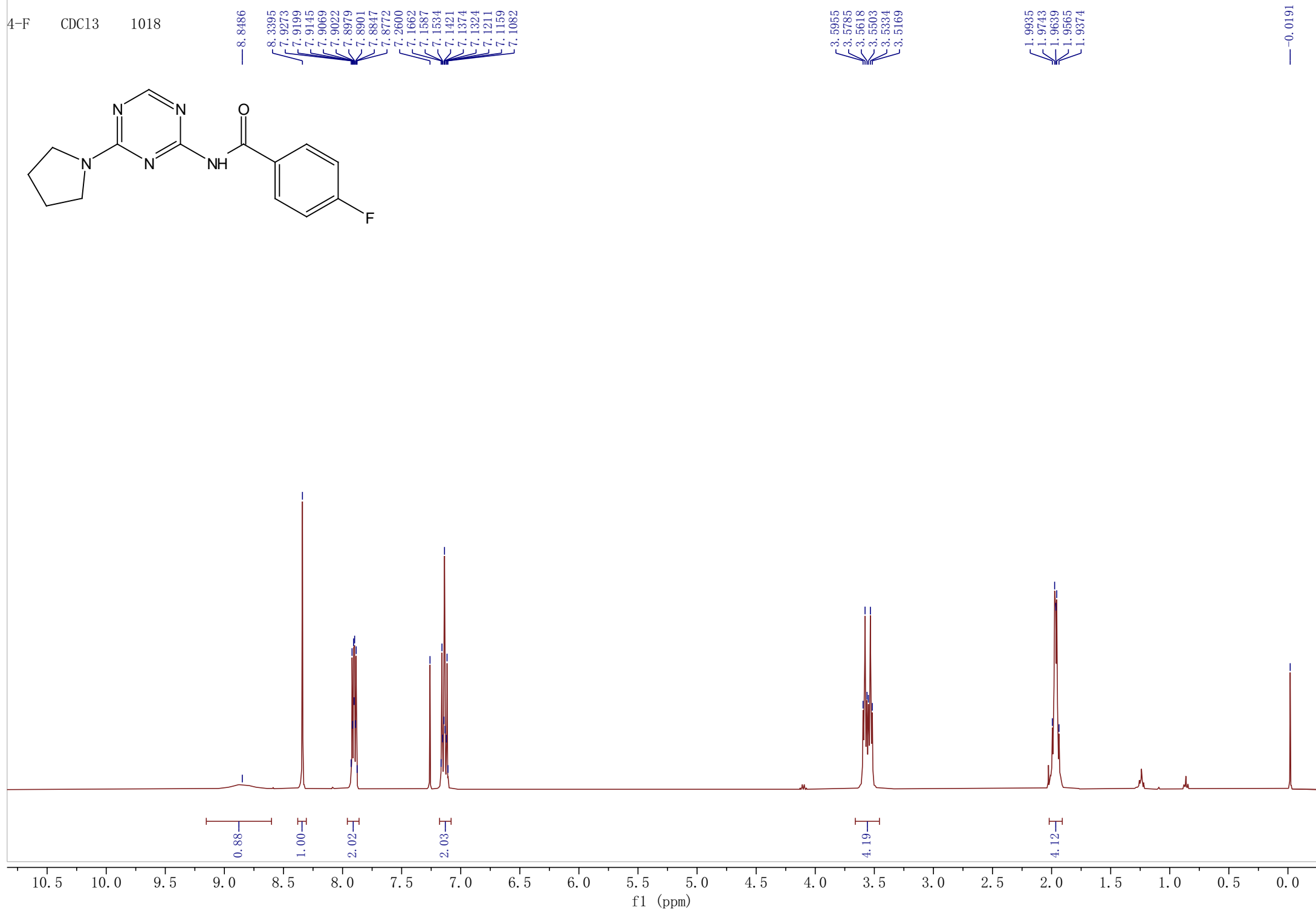
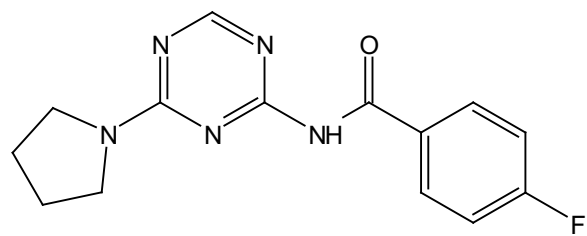
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4-F CDC13 1018



4-F CDC13 1024

166.6313
166.2633
164.8807
164.1088
162.6500
162.4653

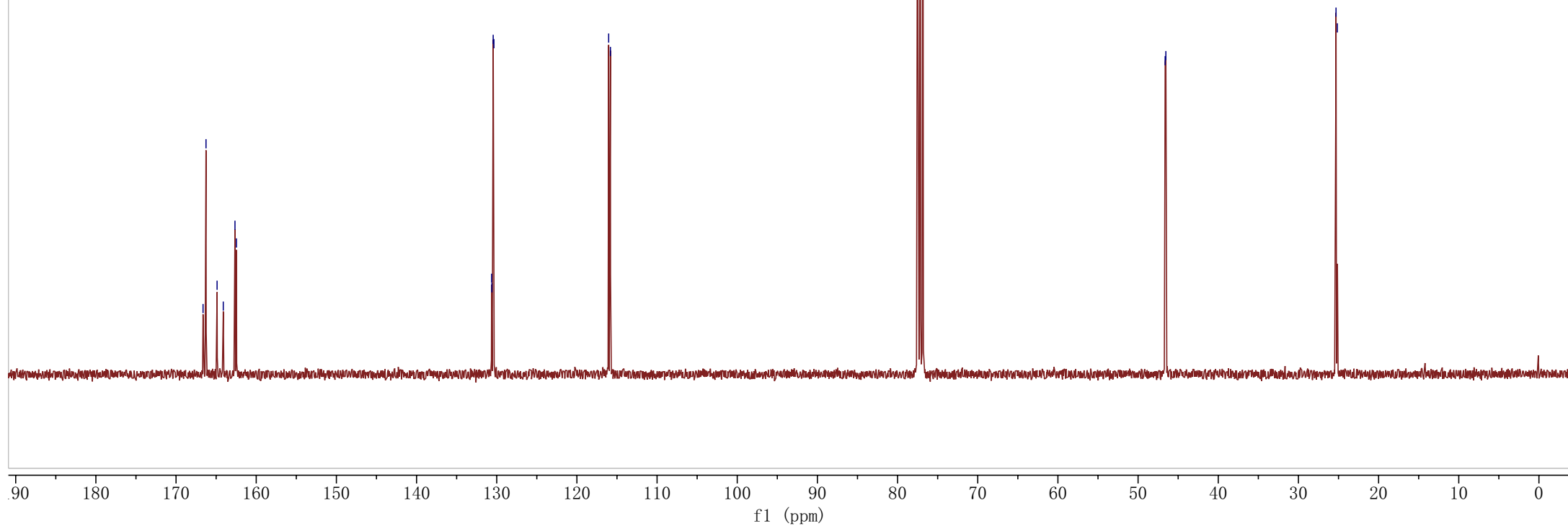
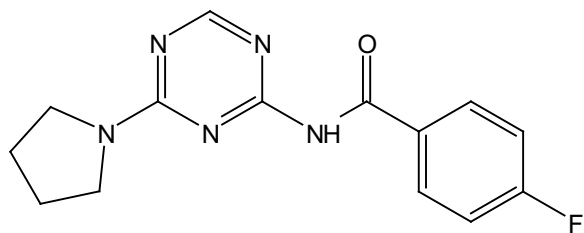
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130.4409
130.3501

116.0376
115.8183

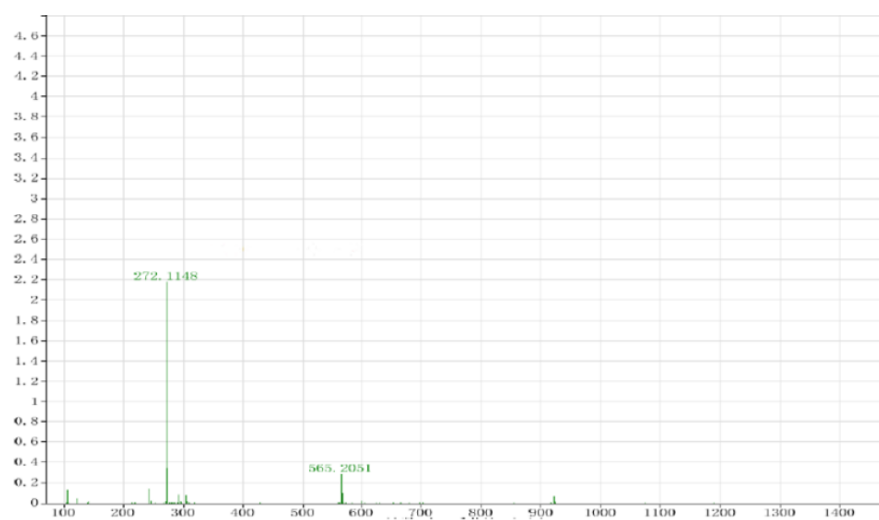
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77.1606
76.8418

46.6231
46.5356

25.3094
25.1471



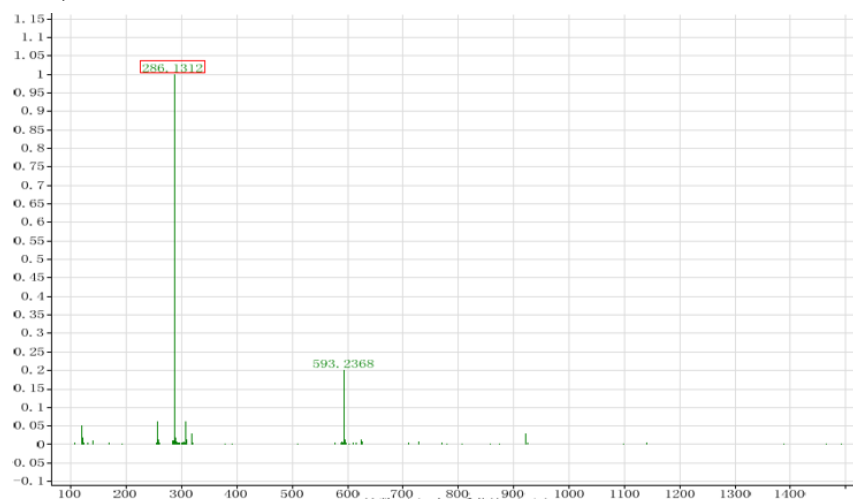
HRMS for compound **3a**



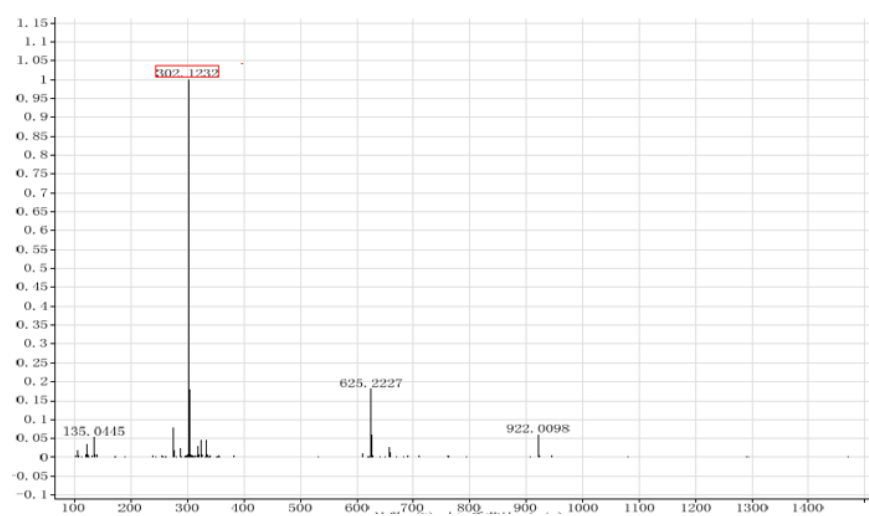
HRMS for compound **3b**



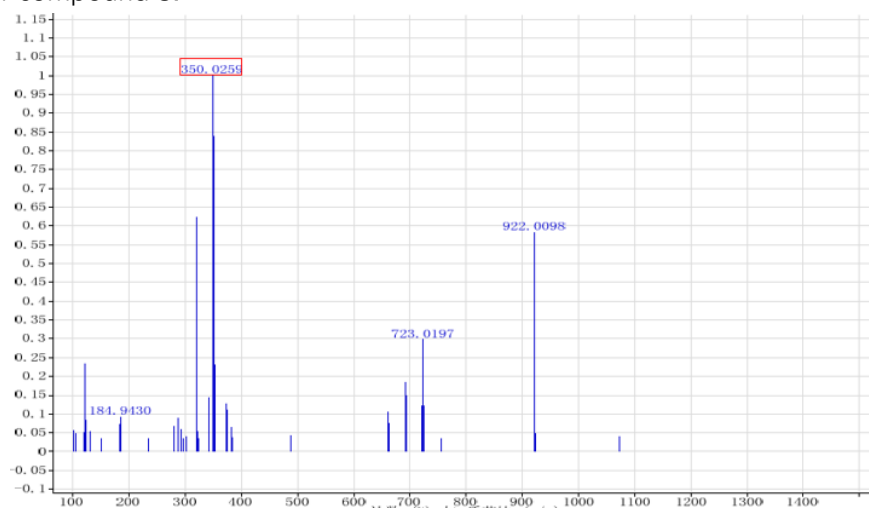
HRMS for compound **3c**



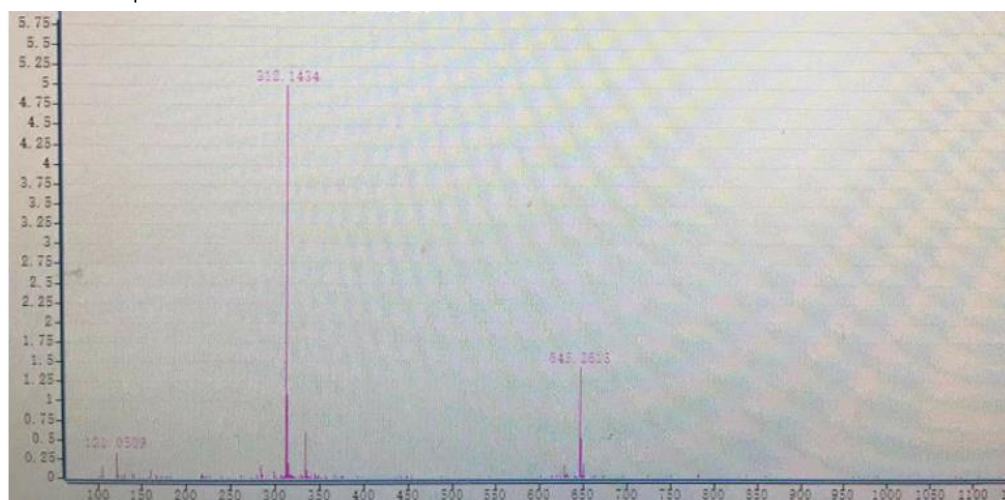
HRMS for compound **3f**



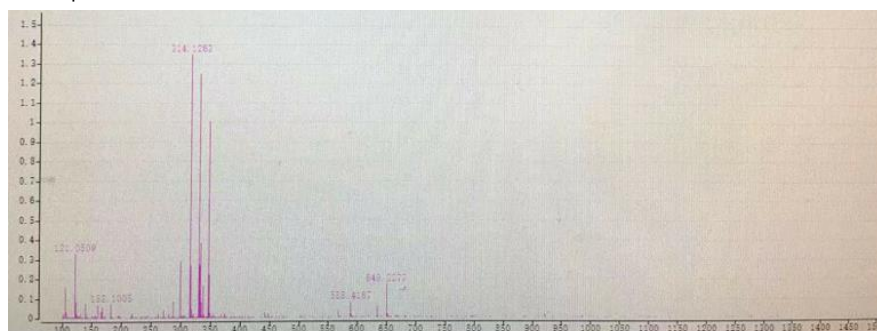
HRMS for compound **3i**



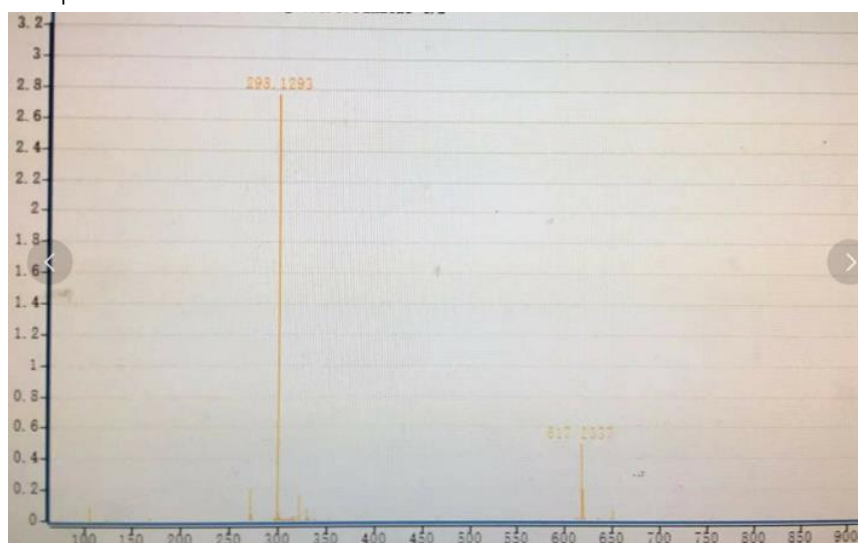
HRMS for compound **3m**



HRMS for compound **3n**



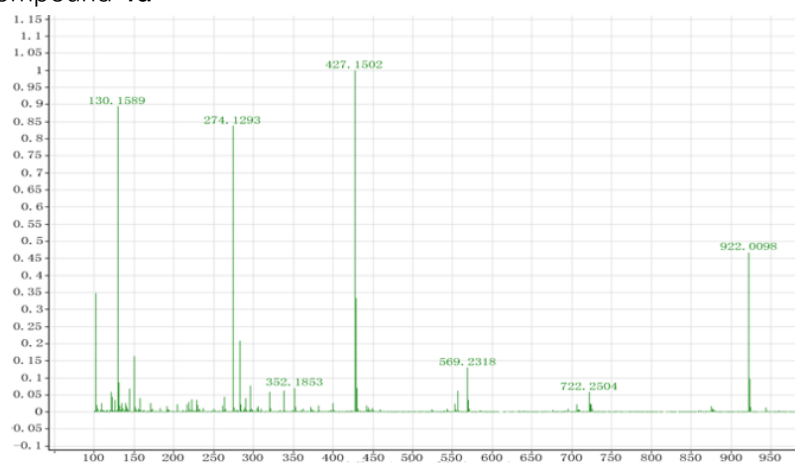
HRMS for compound **3o**



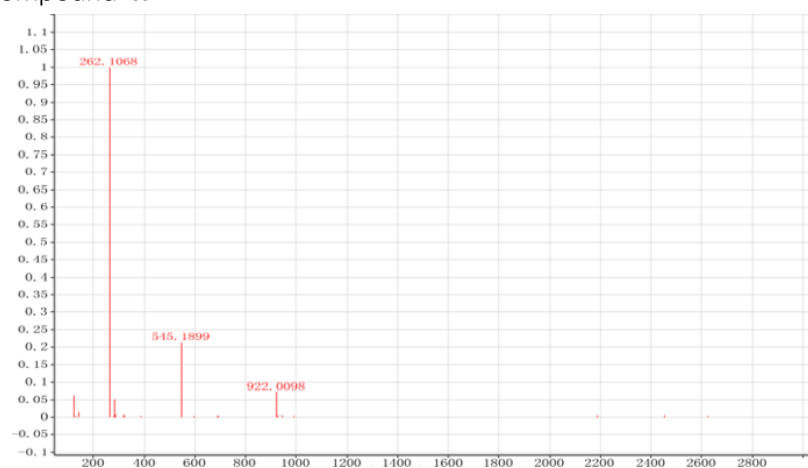
HRMS for compound **4c**



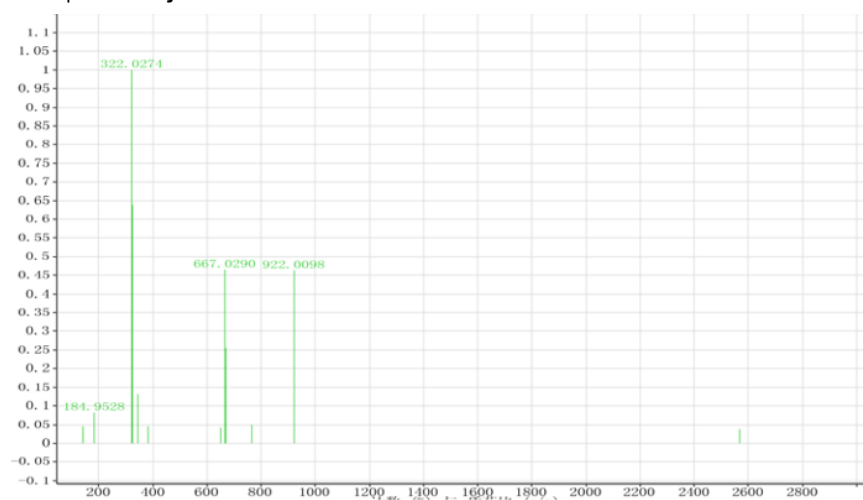
HRMS for compound **4d**



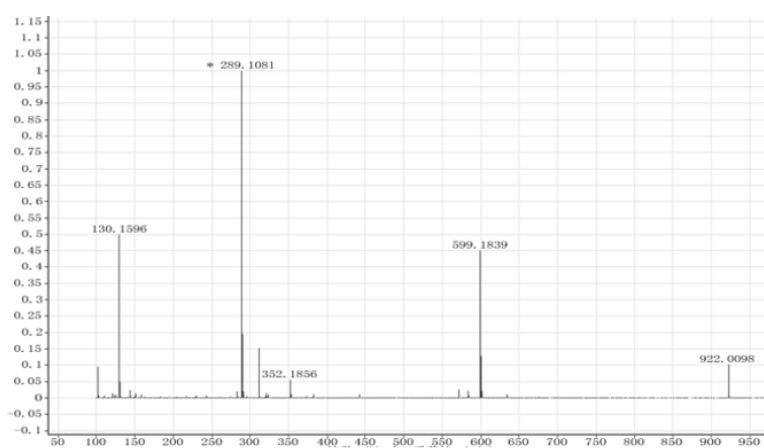
HRMS for compound **4f**



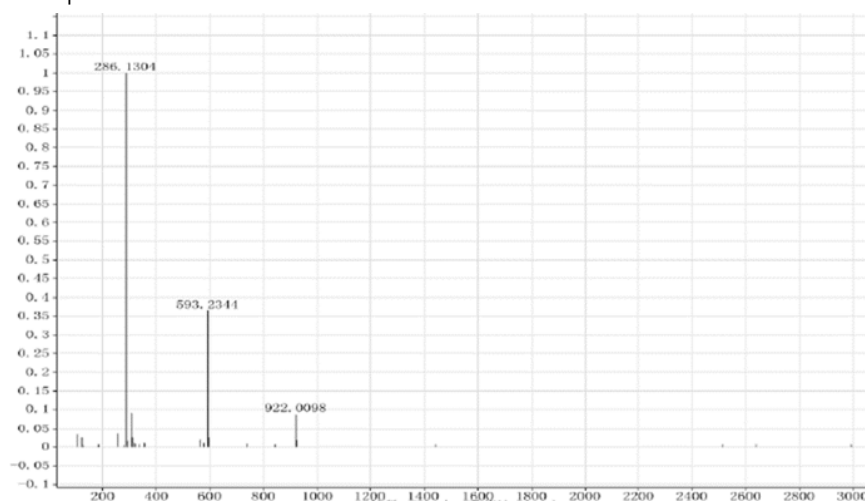
HRMS for compound **4j**



HRMS for compound **4k**



HRMS for compound **4m**



HRMS for compound **4n**

