Support information

One-pot Synthesis of 2-Amino-4(3*H*)-Quinazolinones via Ring-opening of Isatoic anhydride with amines and Palladium-catalyzed Oxidative Isocyanide-insertion

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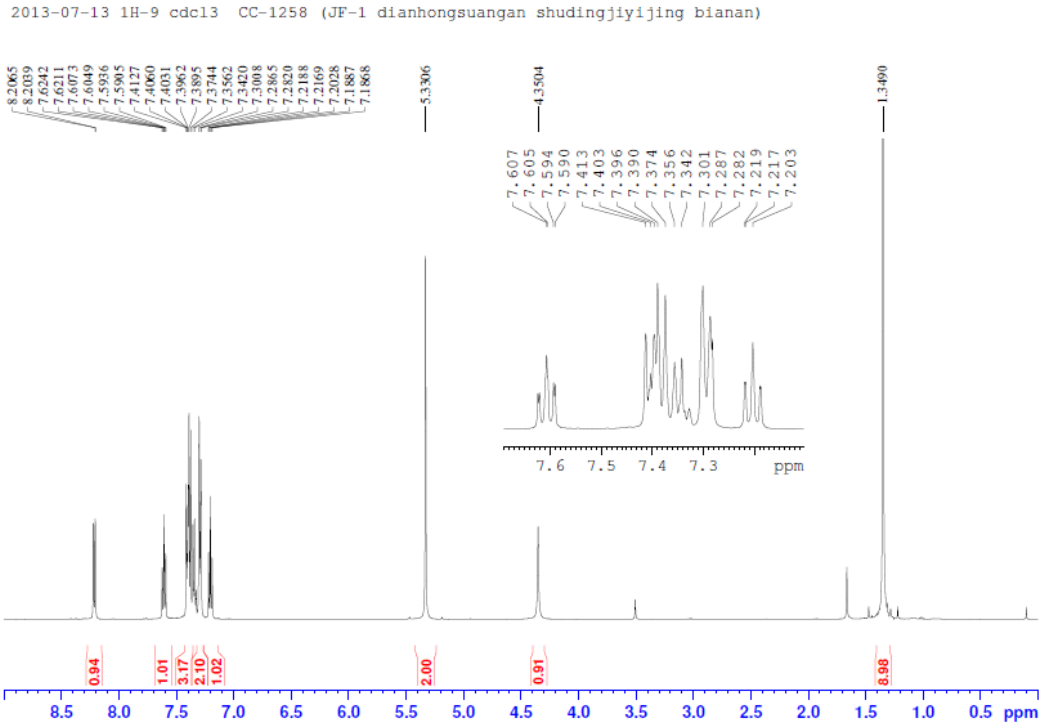
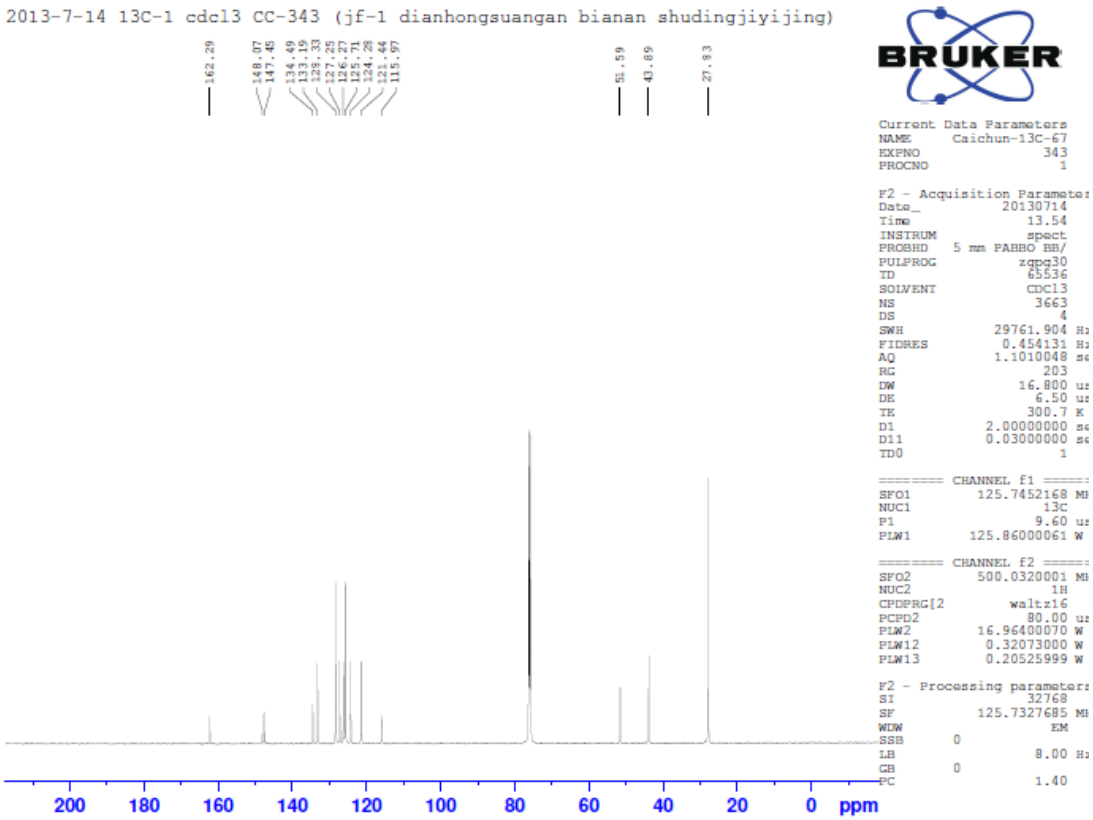
Copies of ^{1}H, ^{13}C NMR



^{1}H NMR of compound **4a**



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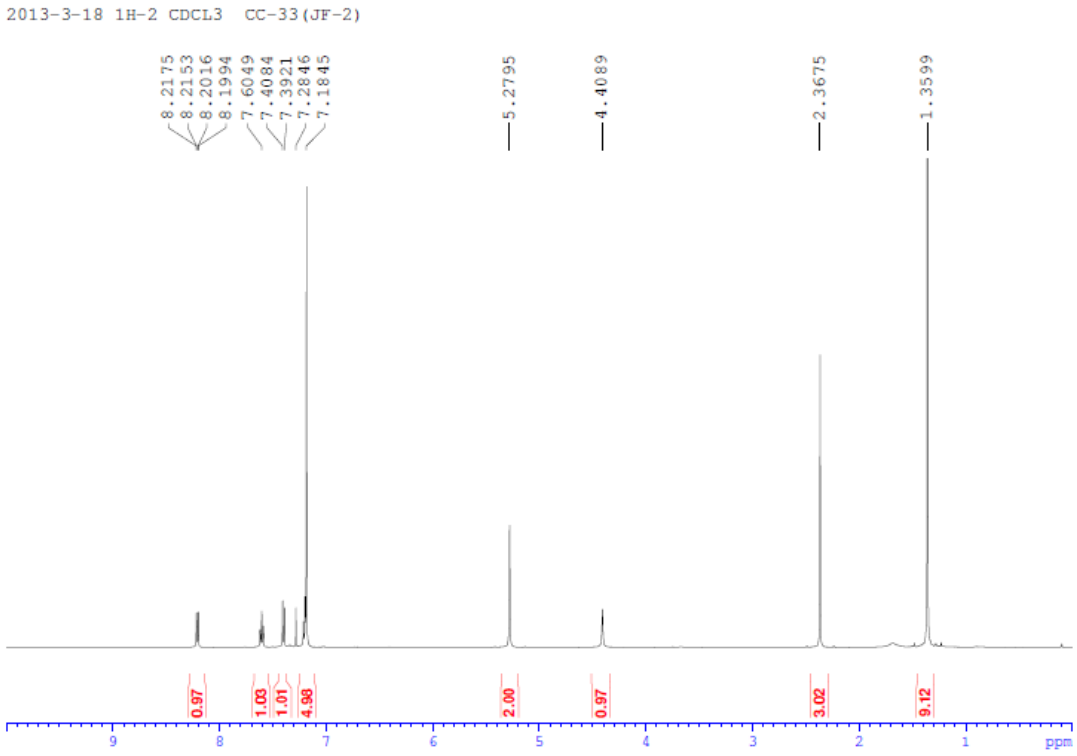

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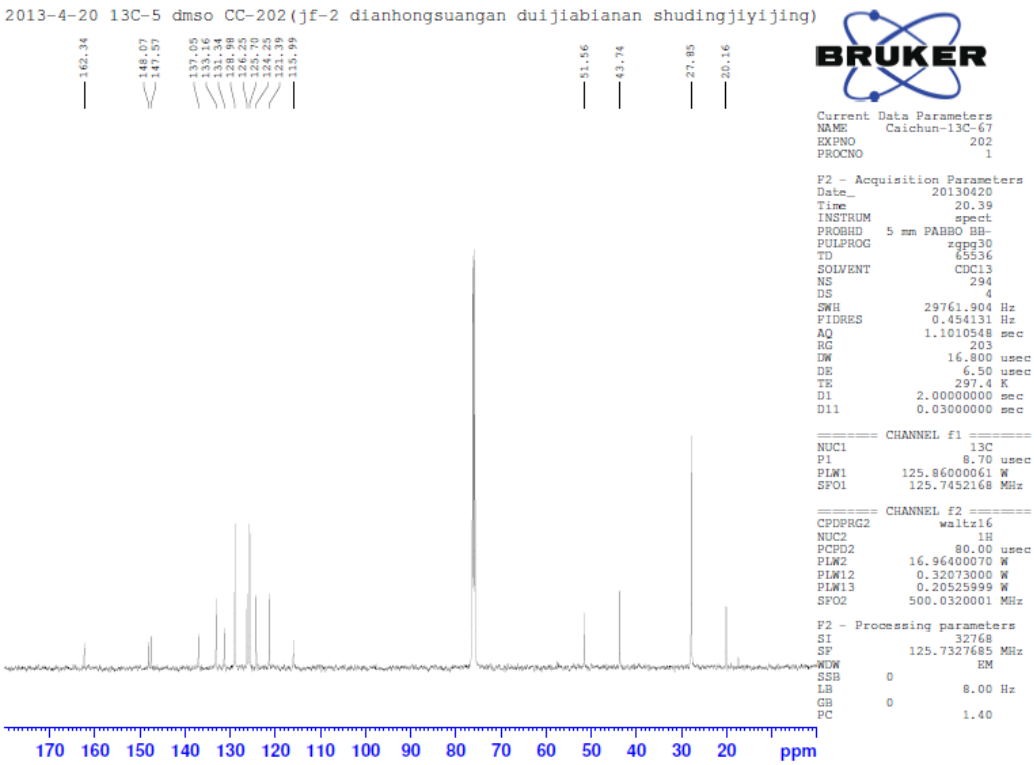

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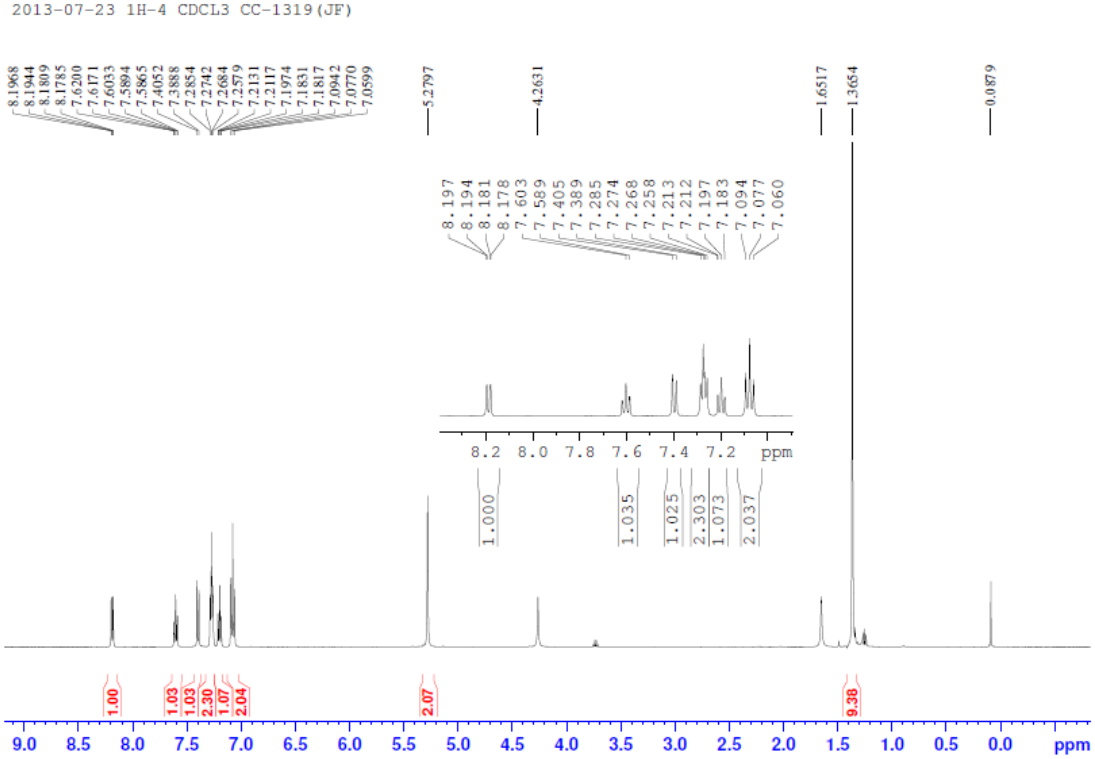

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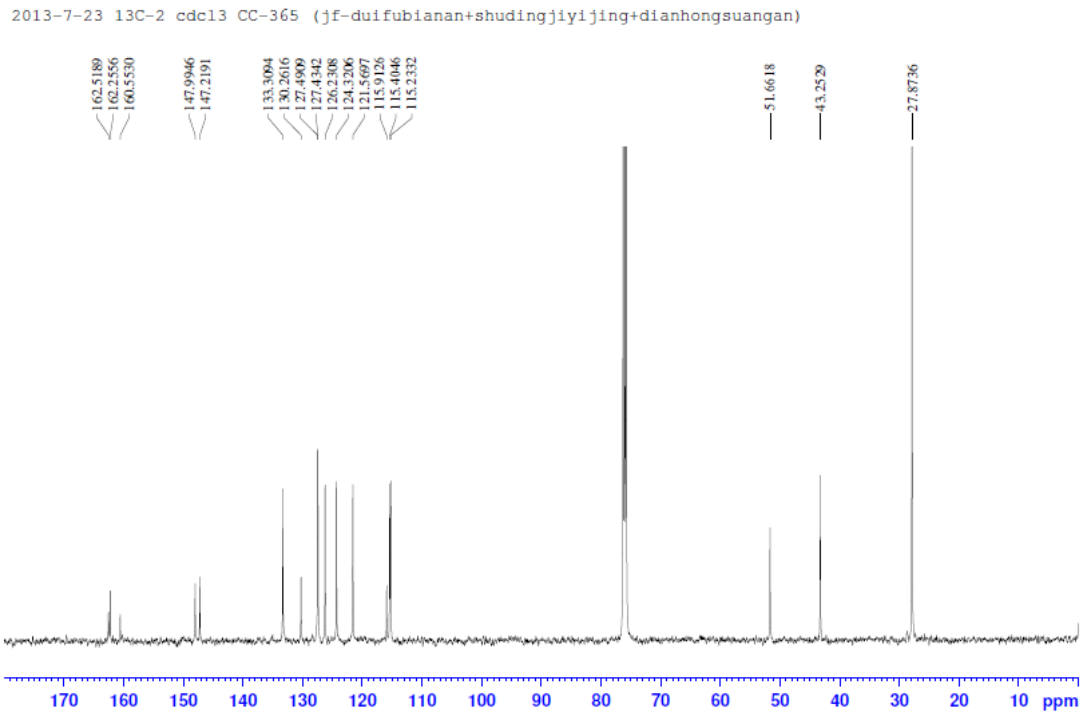

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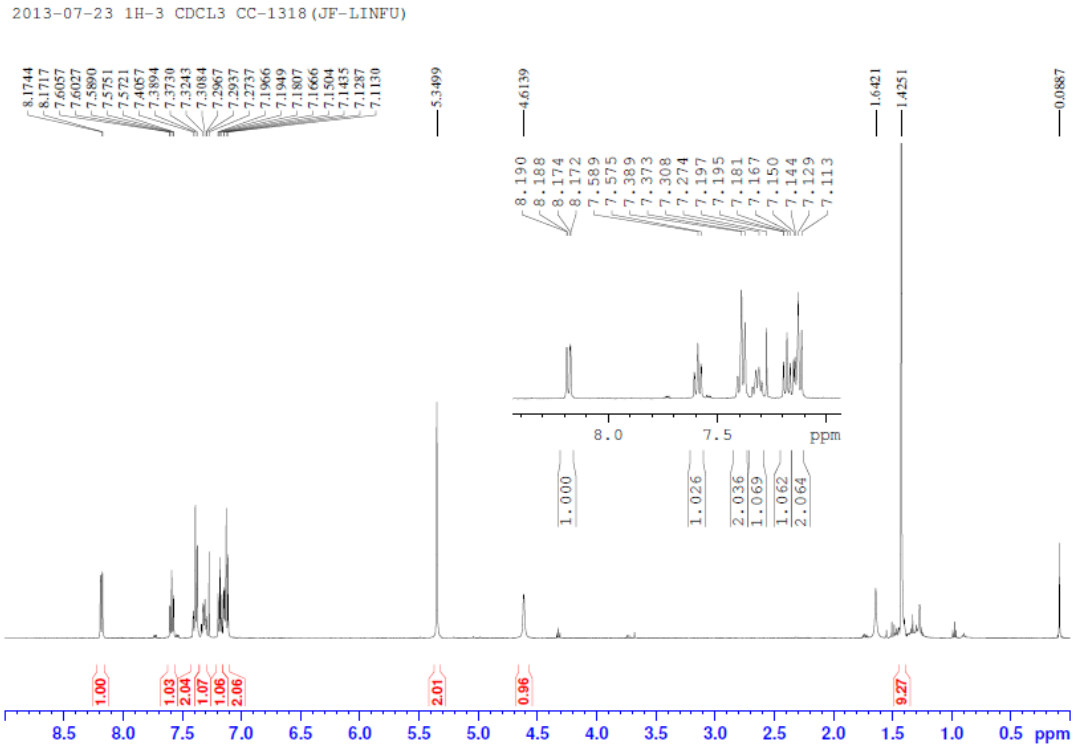

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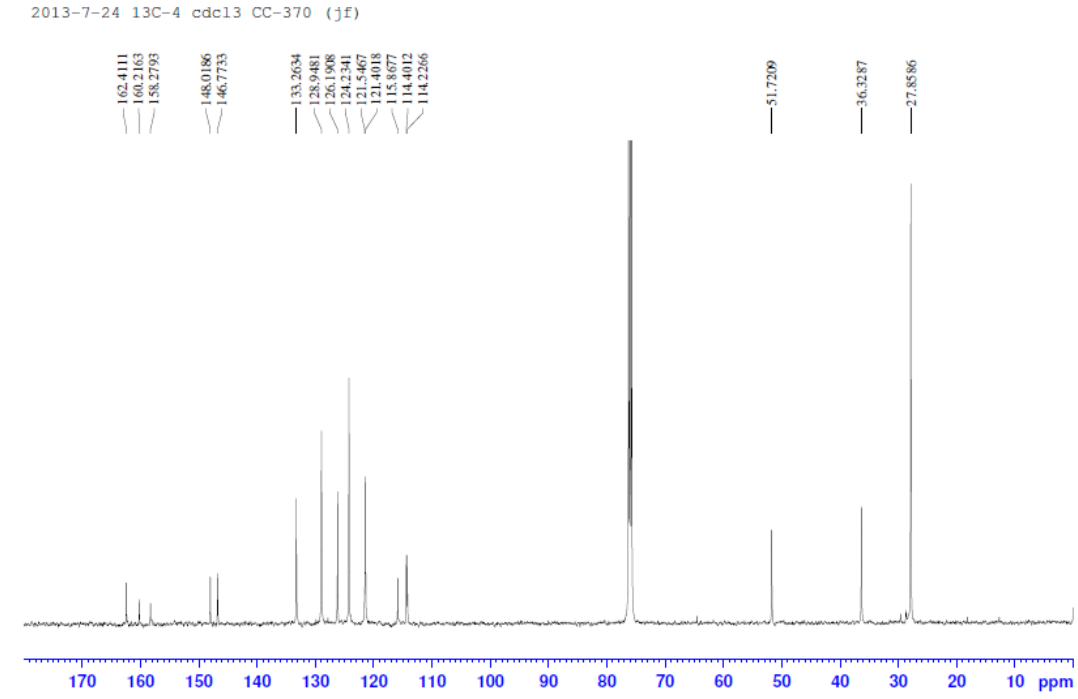

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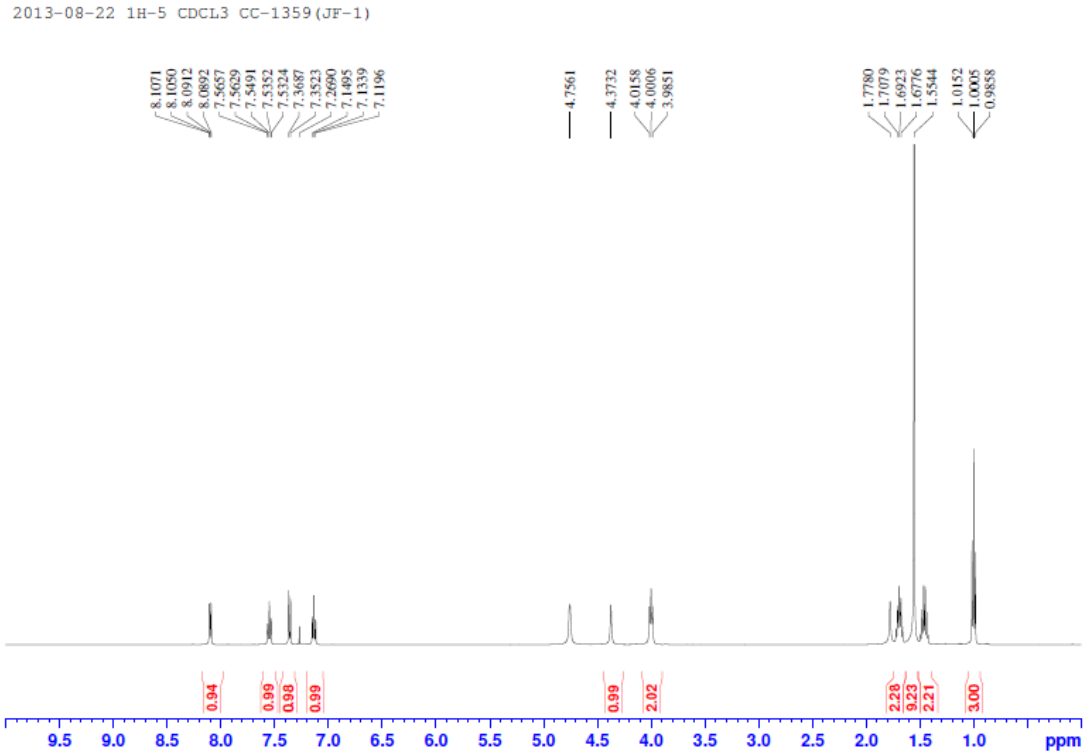

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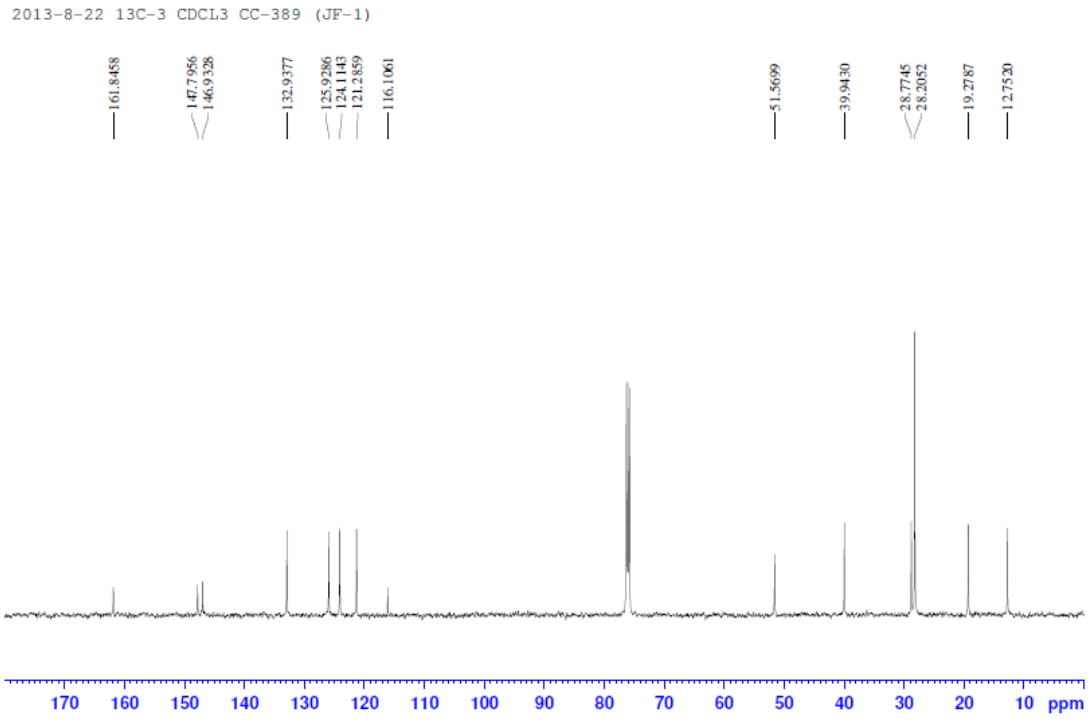

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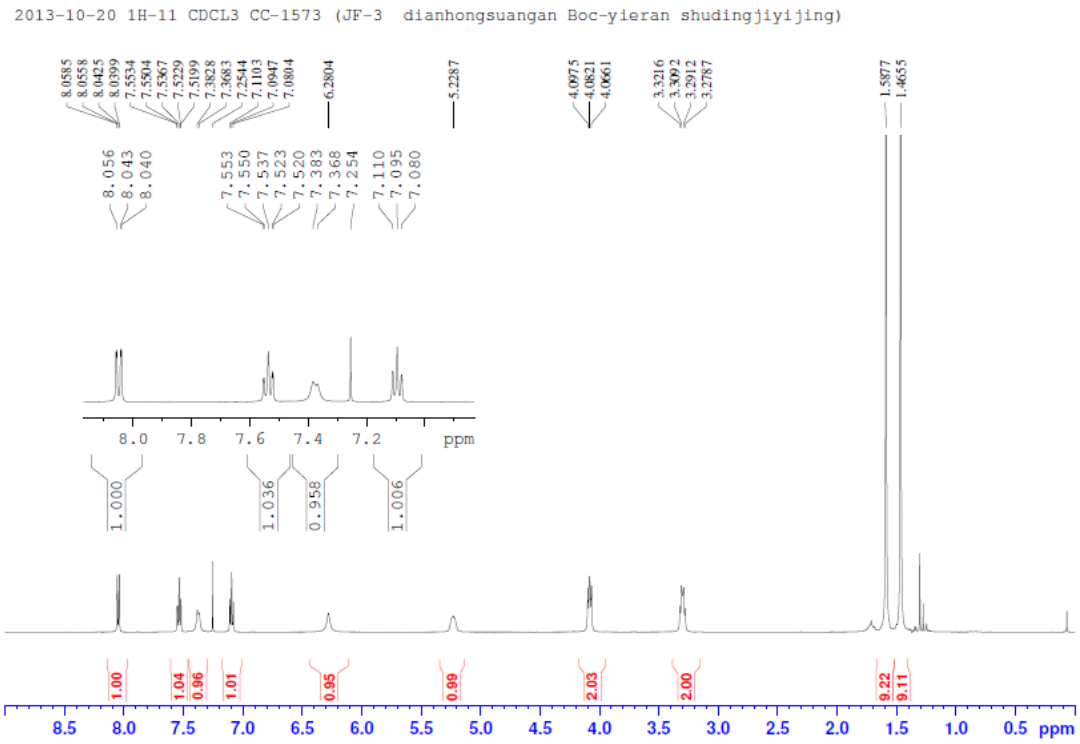

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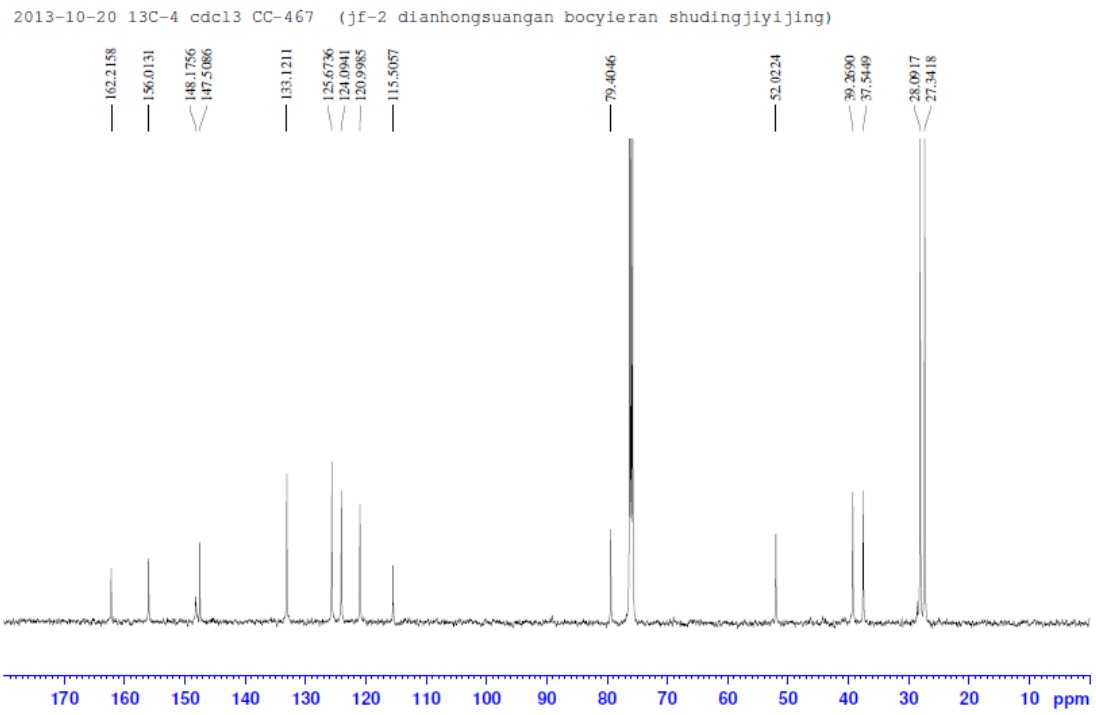

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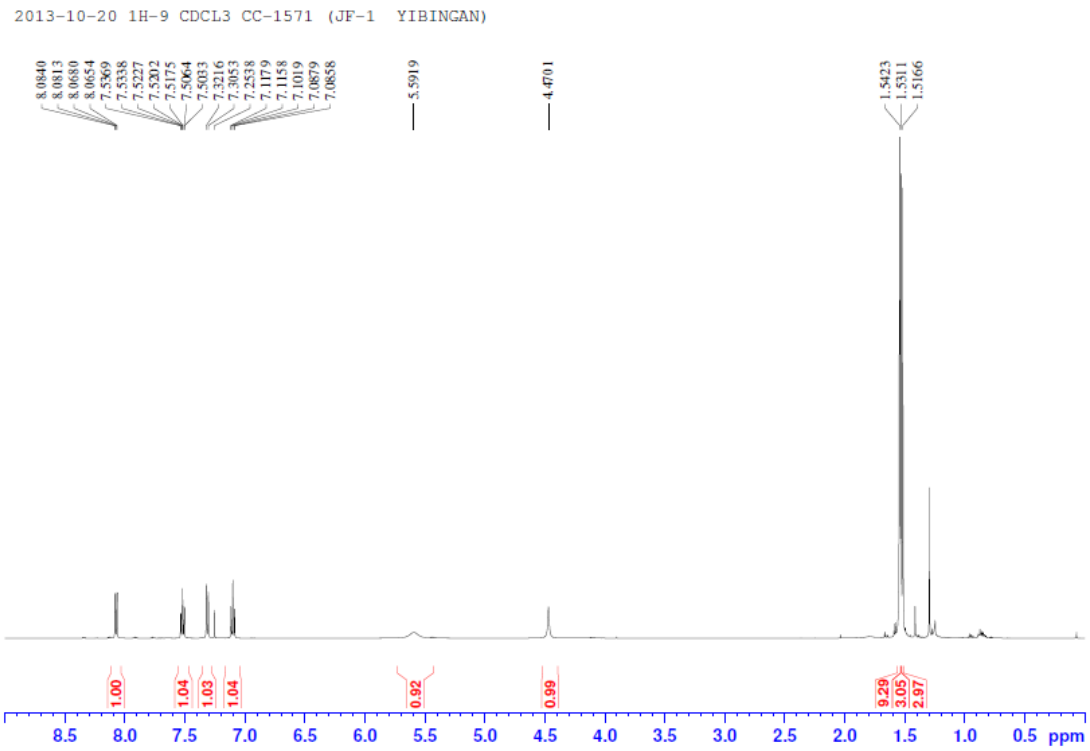

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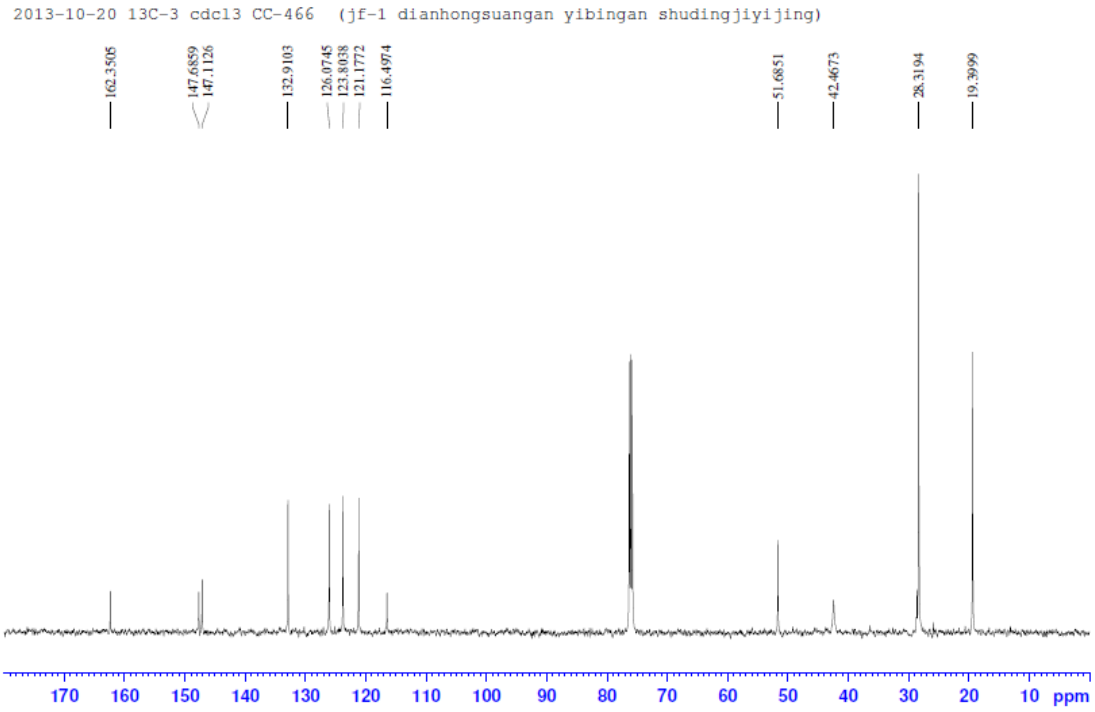

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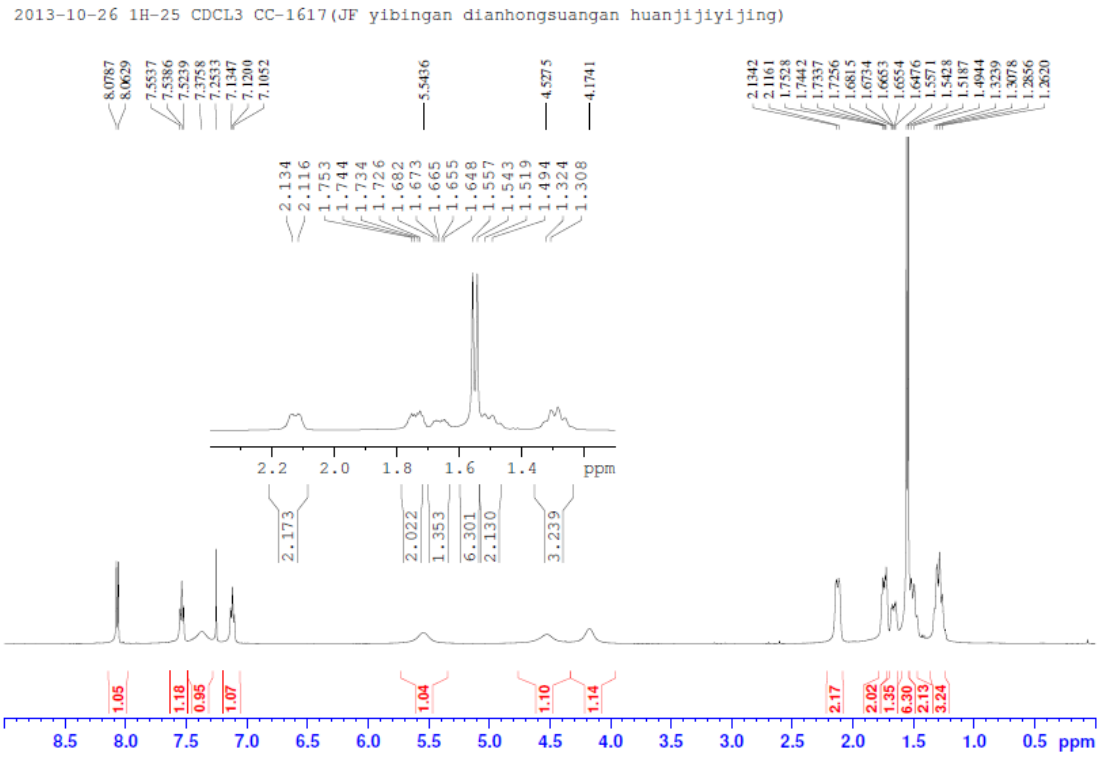

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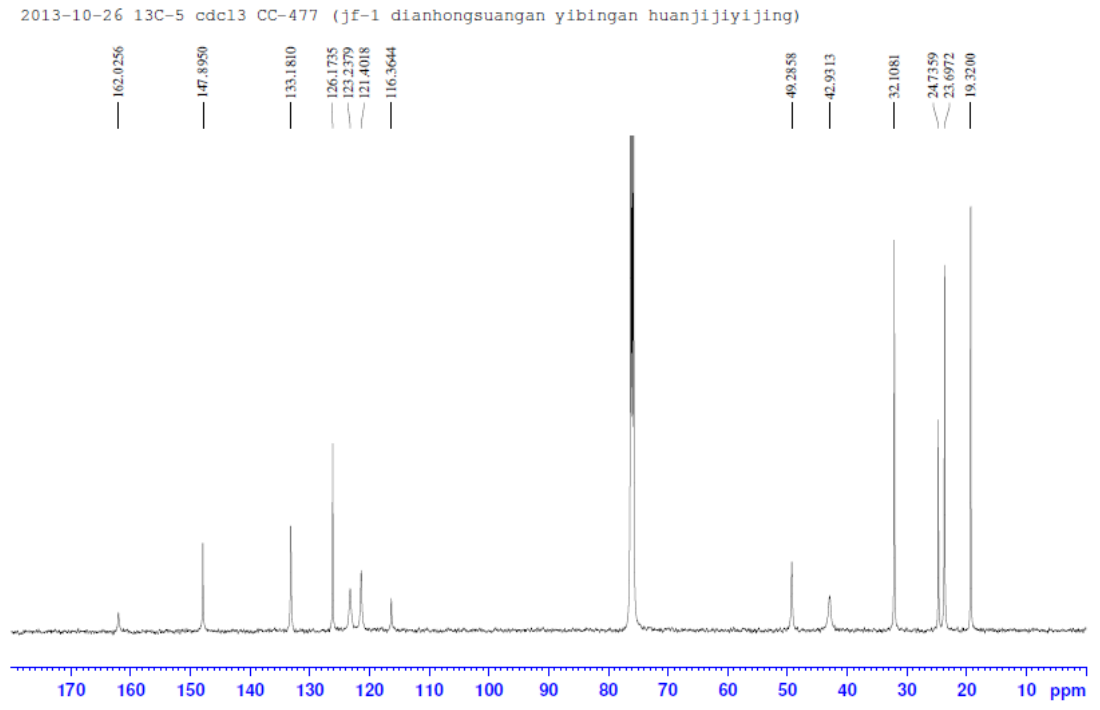

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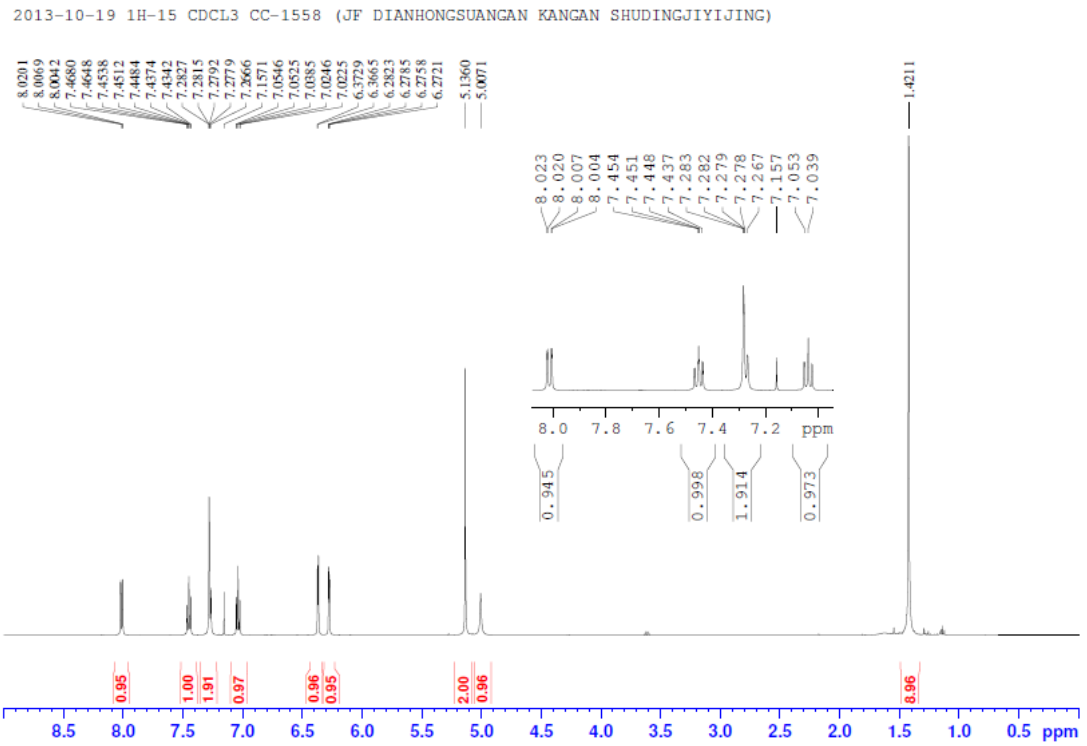

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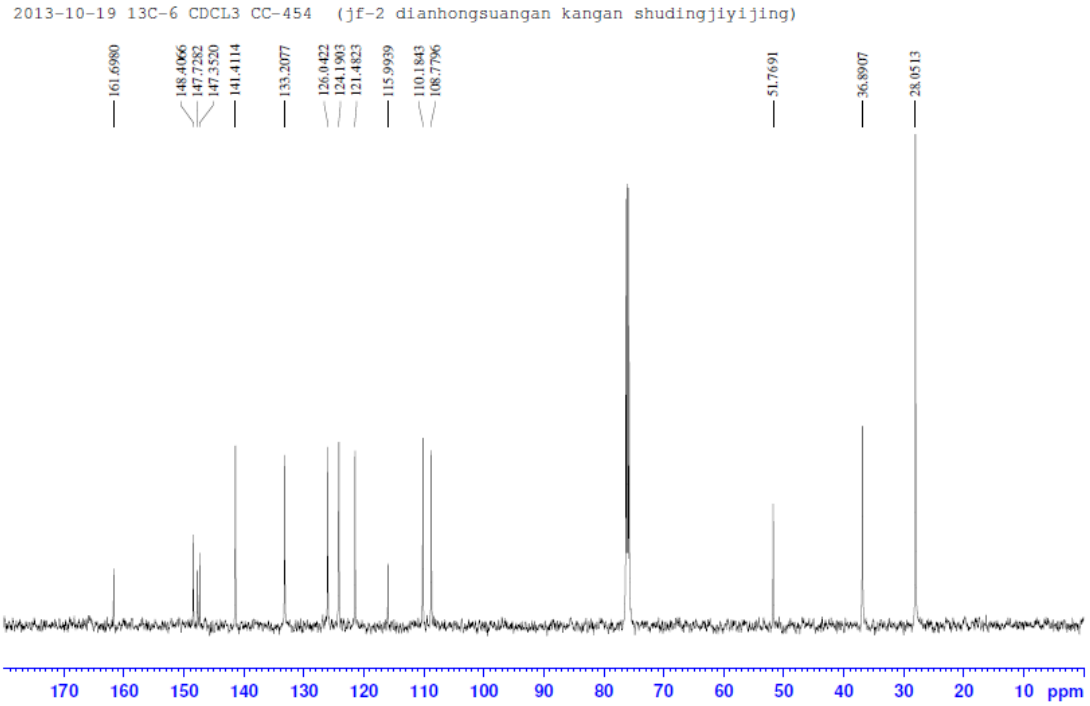

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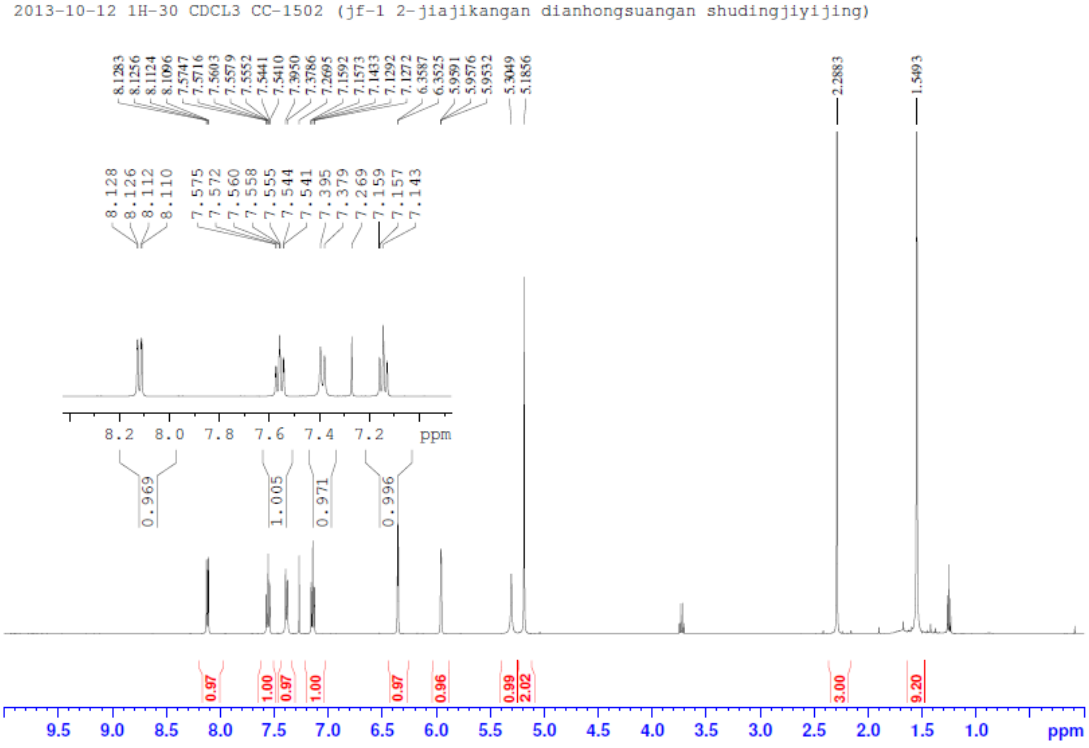

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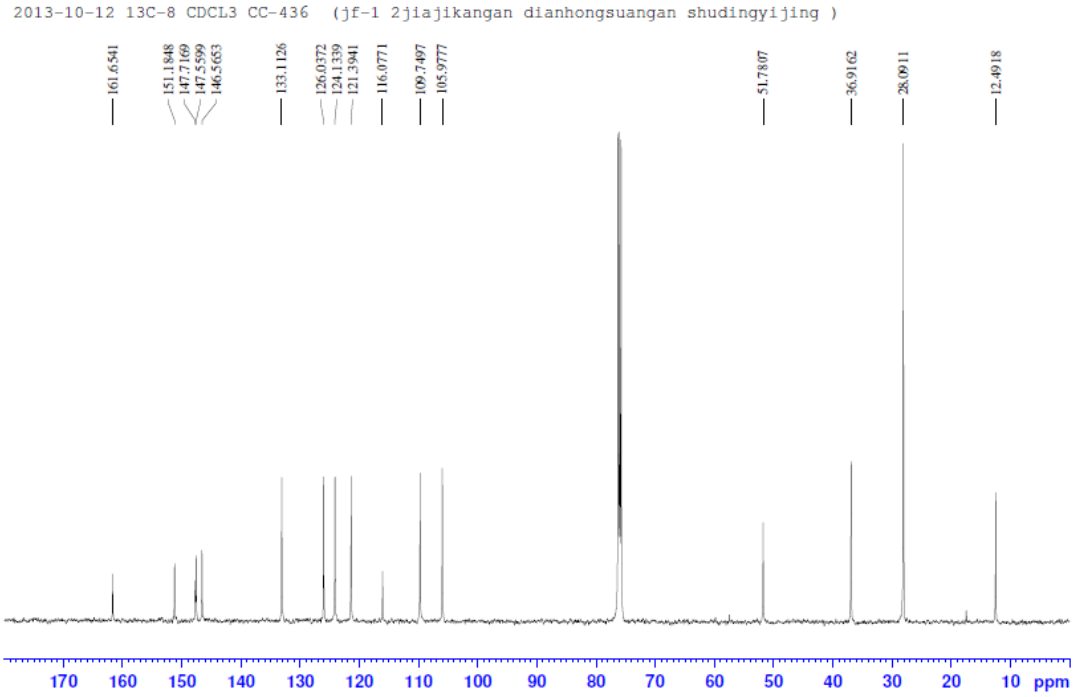

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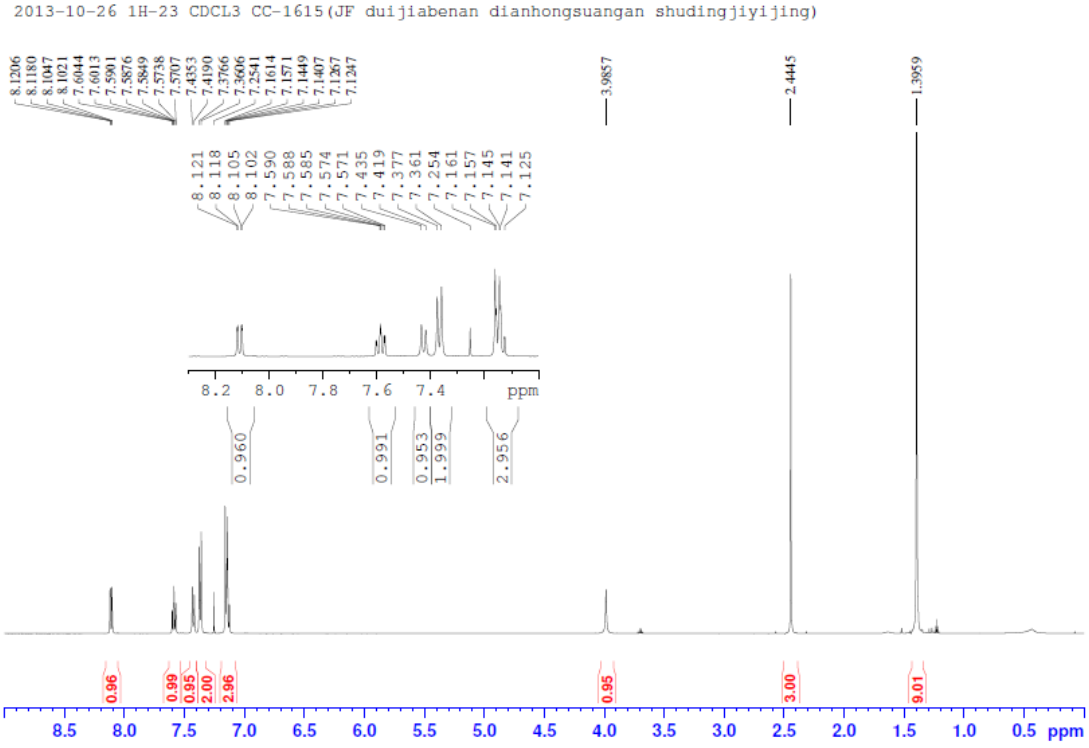

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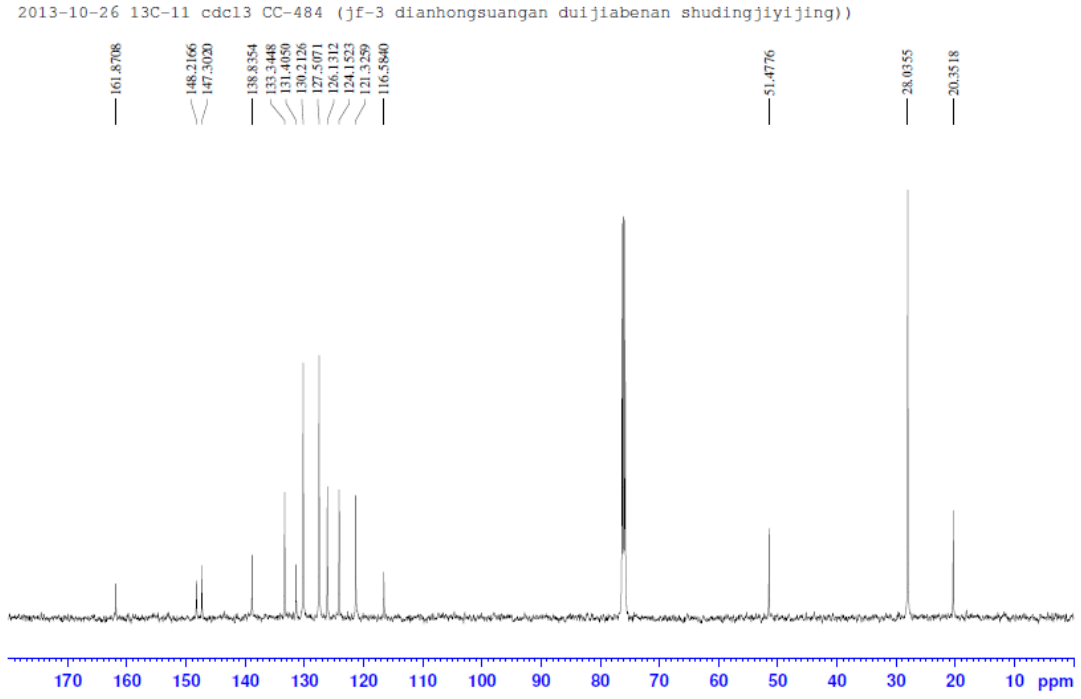

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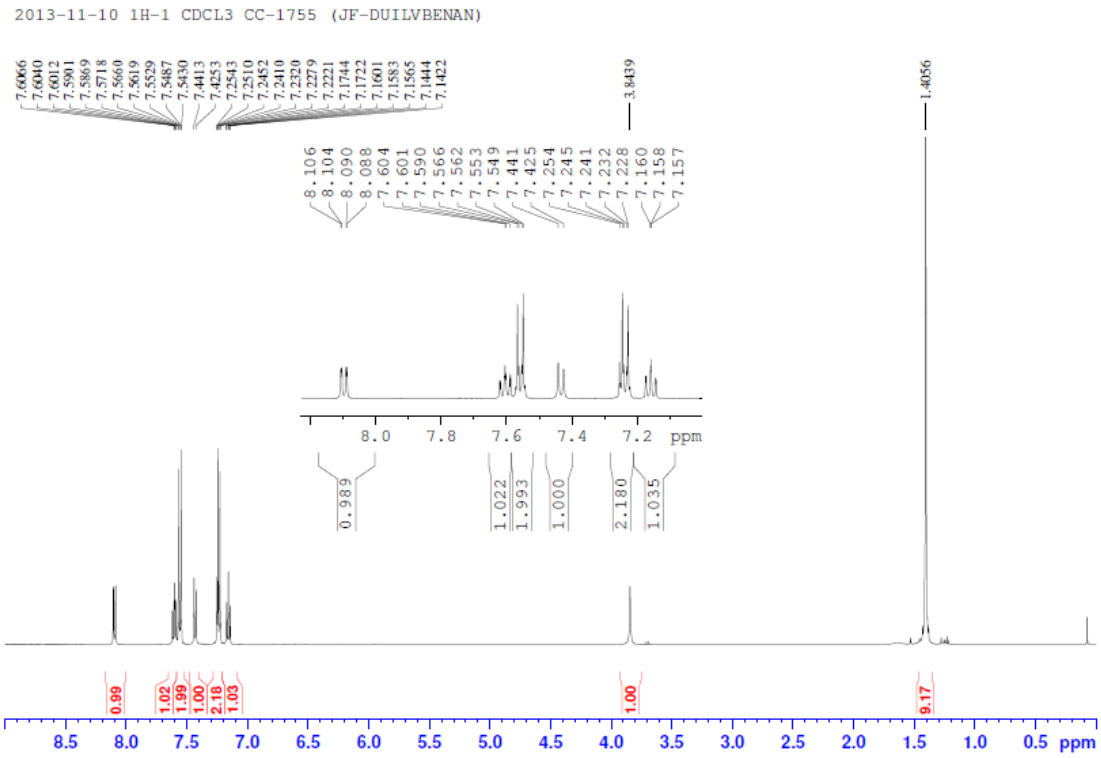

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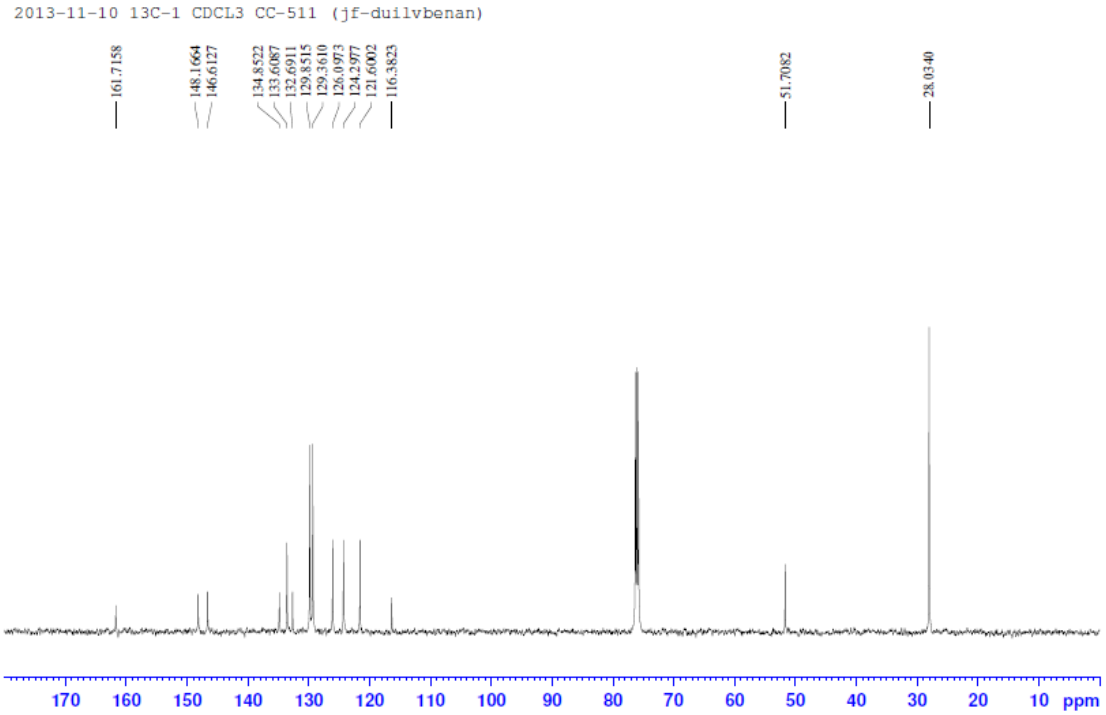

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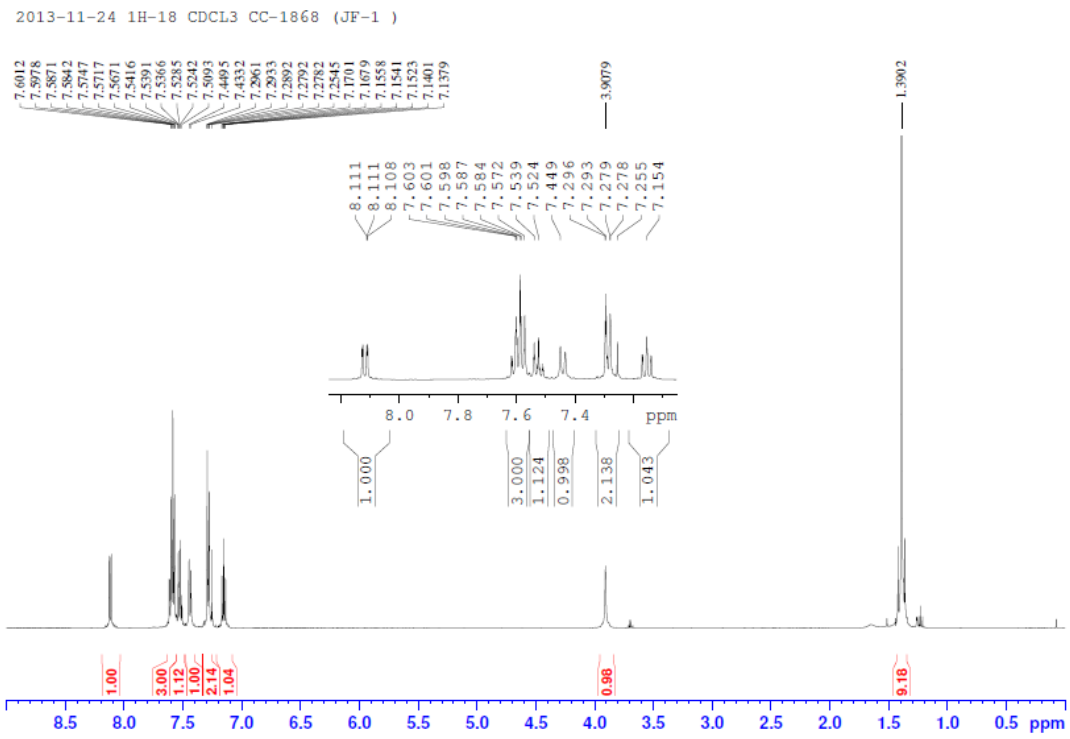

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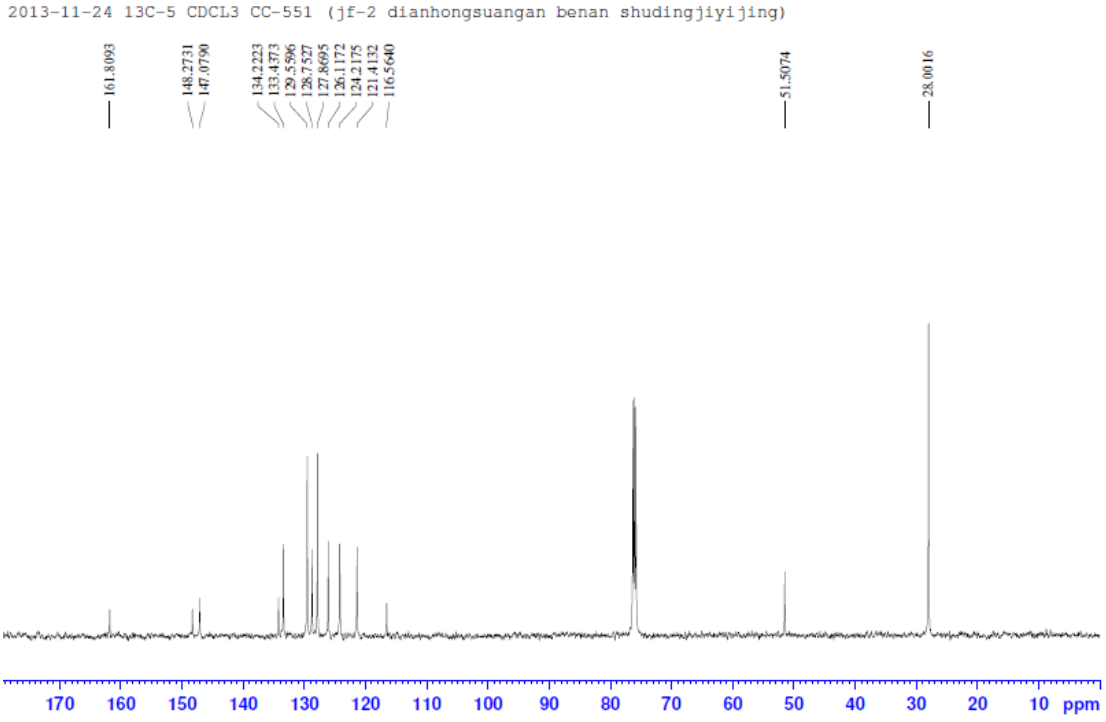

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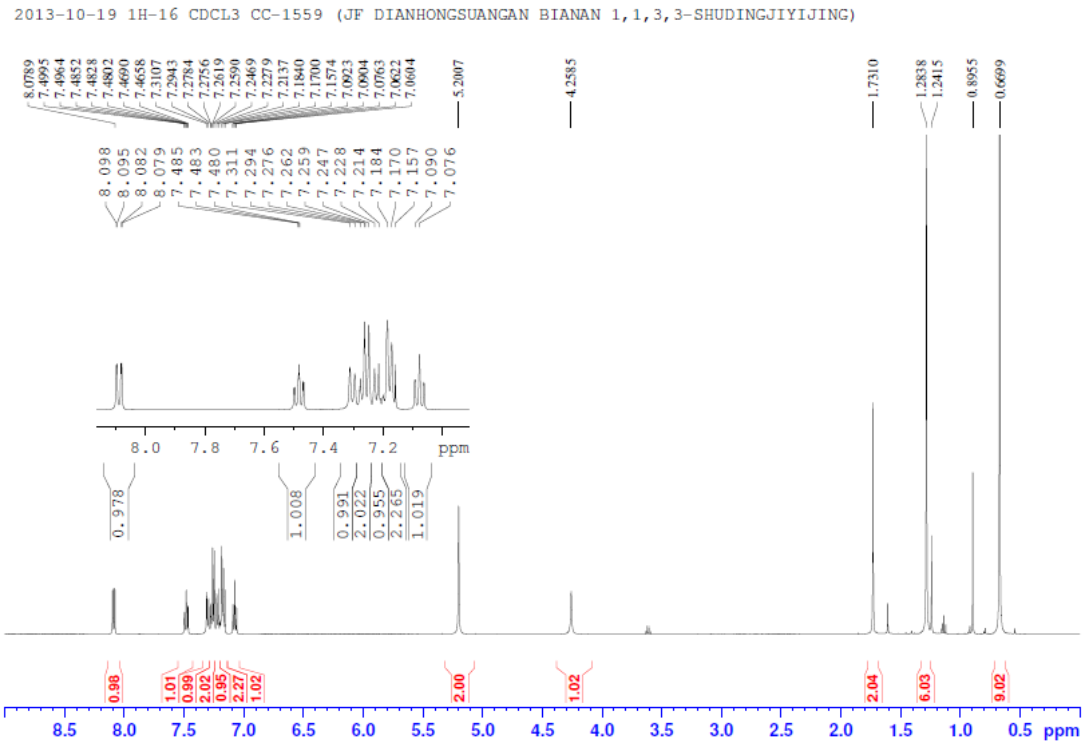

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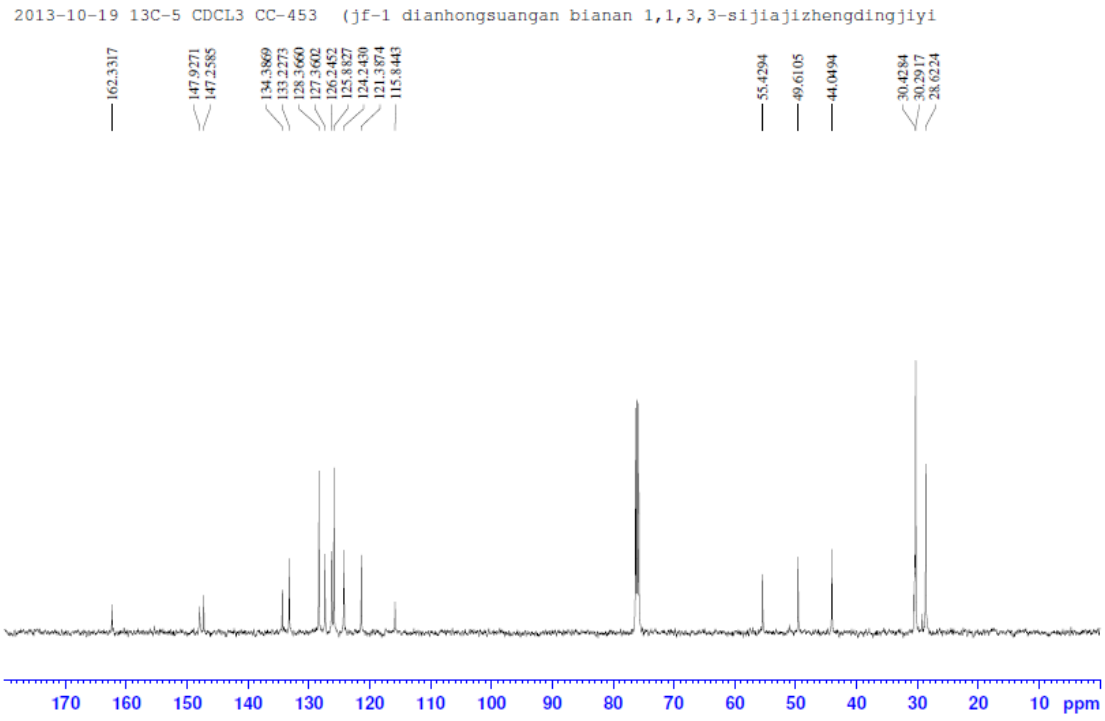

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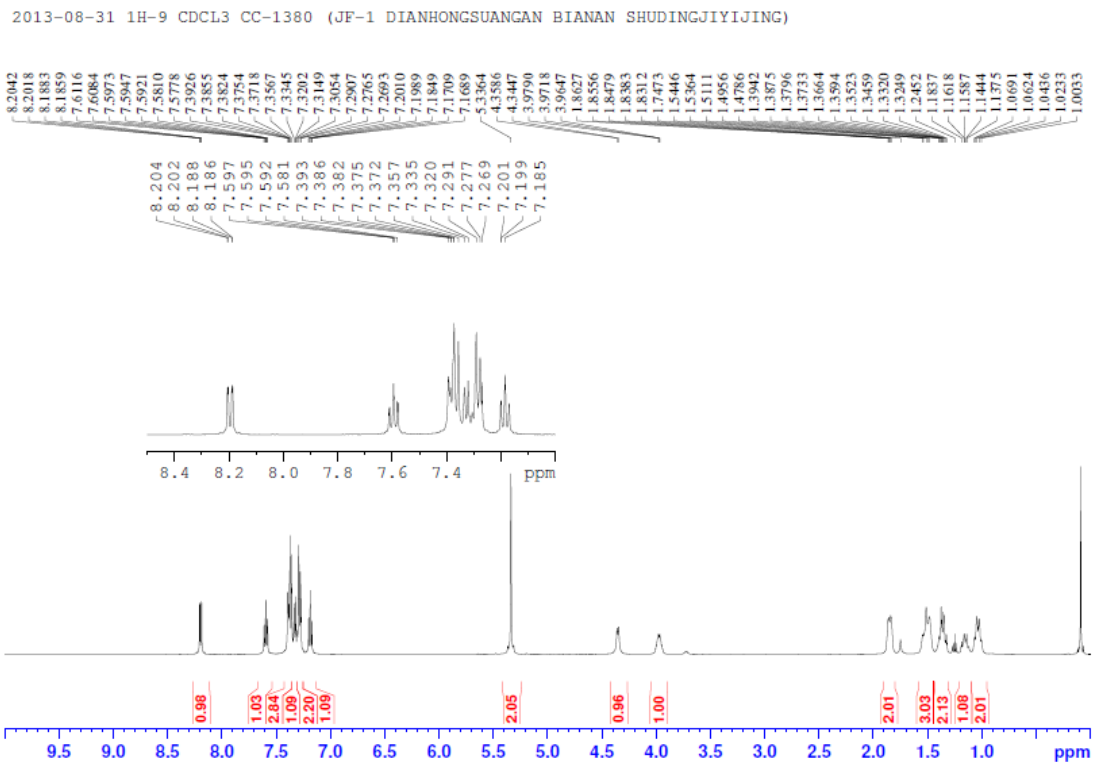

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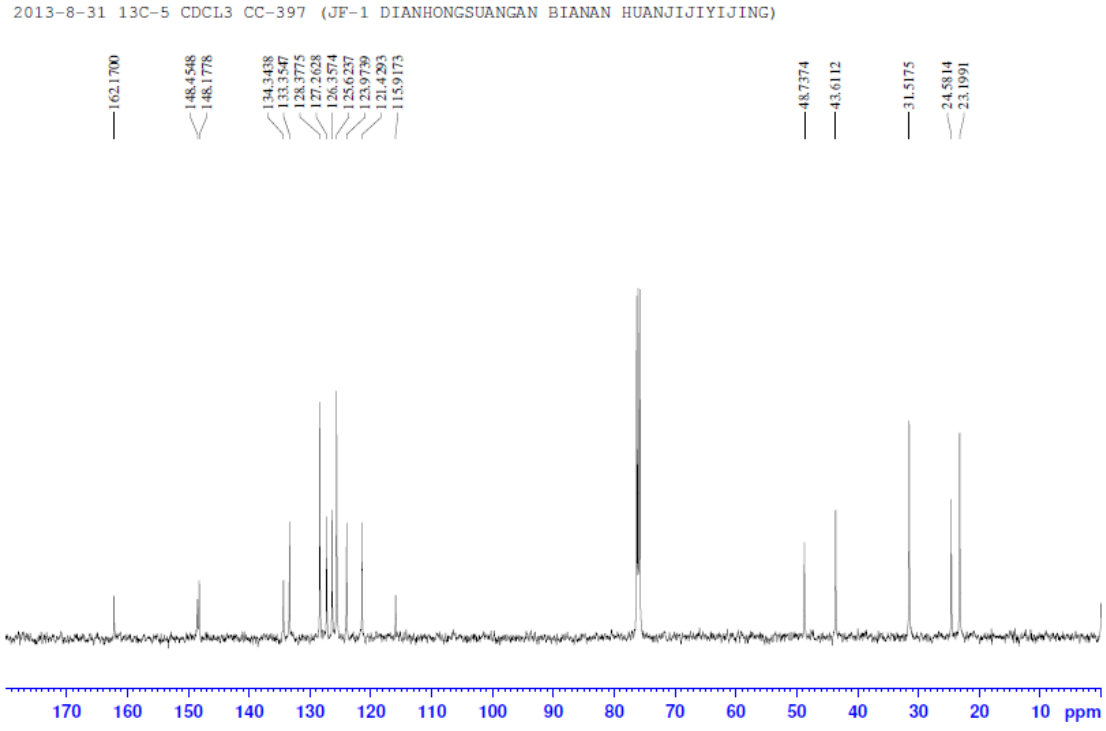

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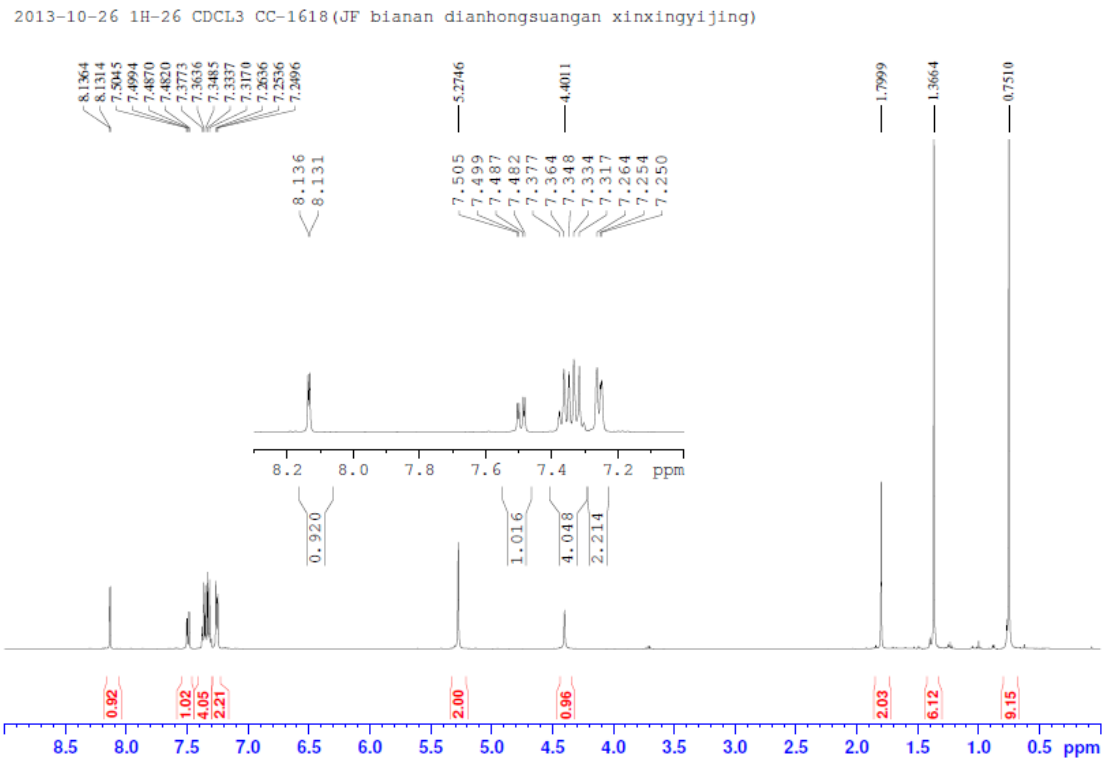

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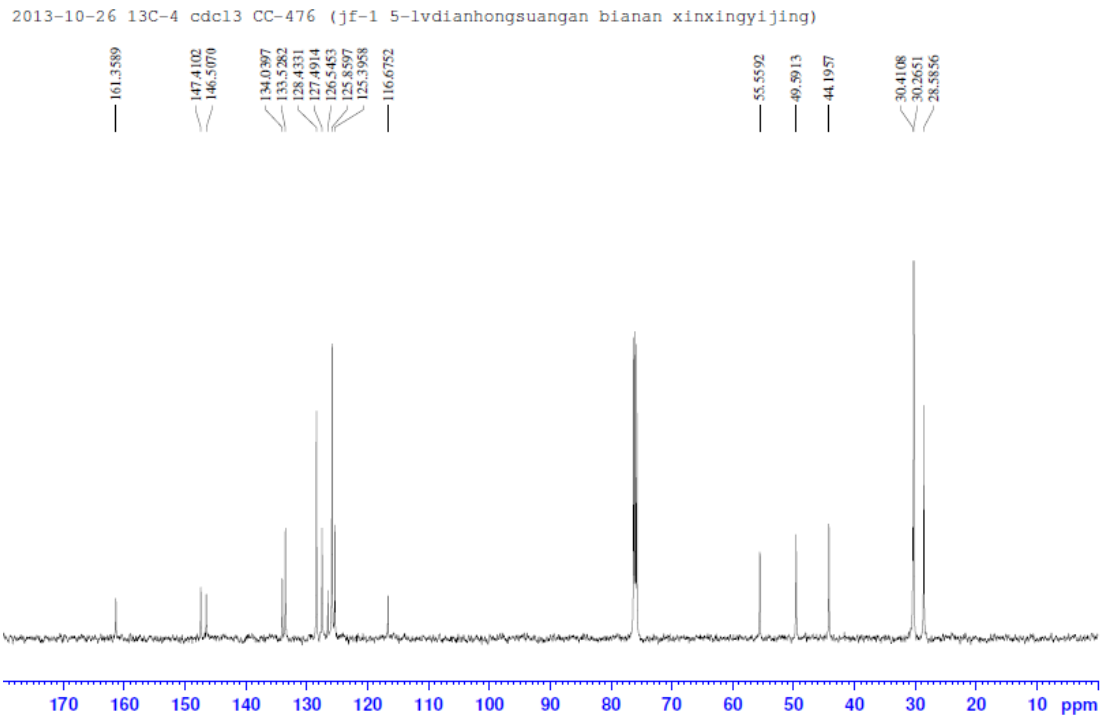

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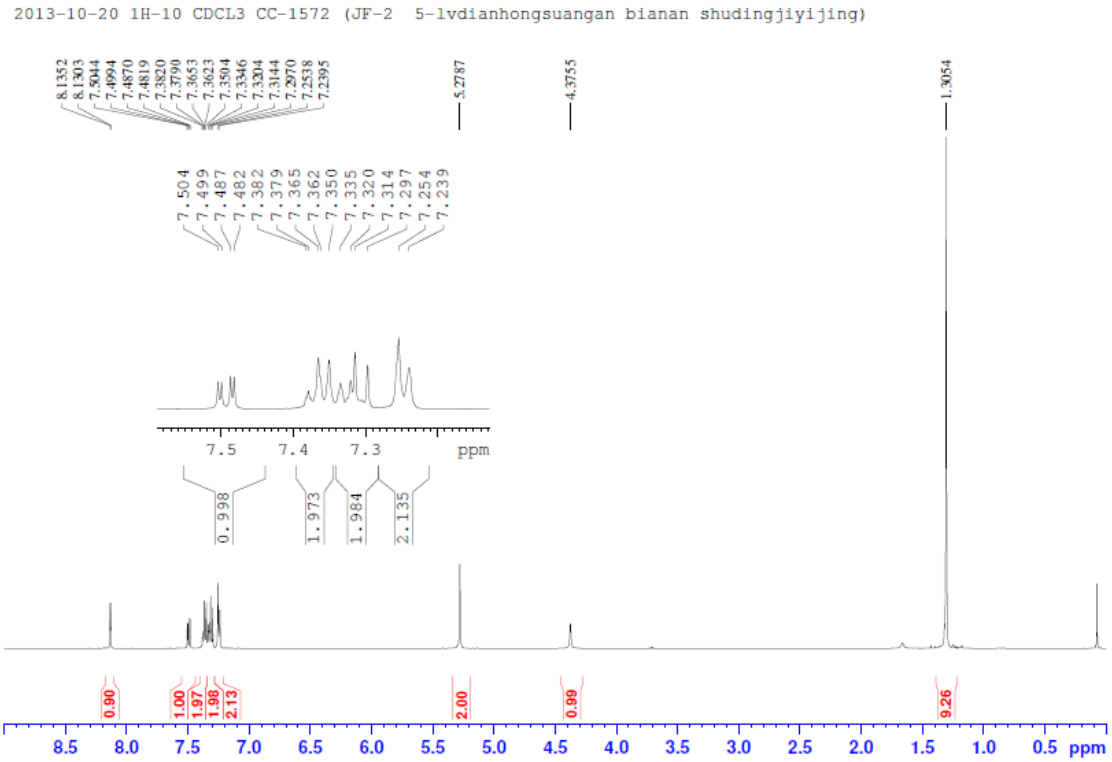

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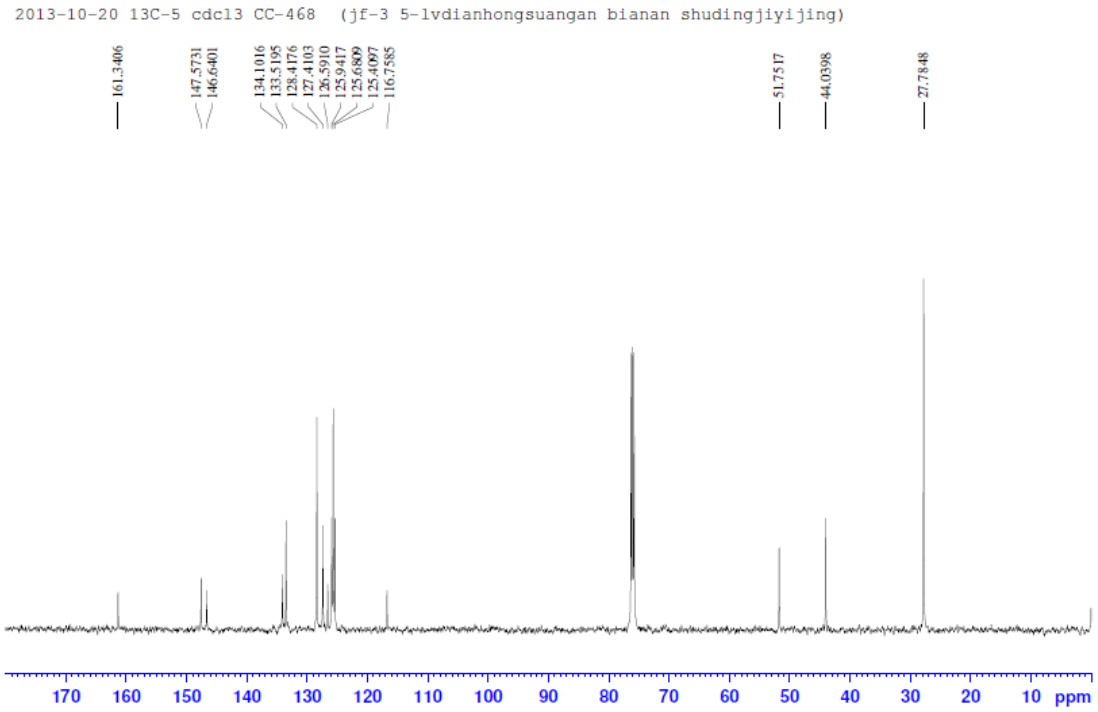

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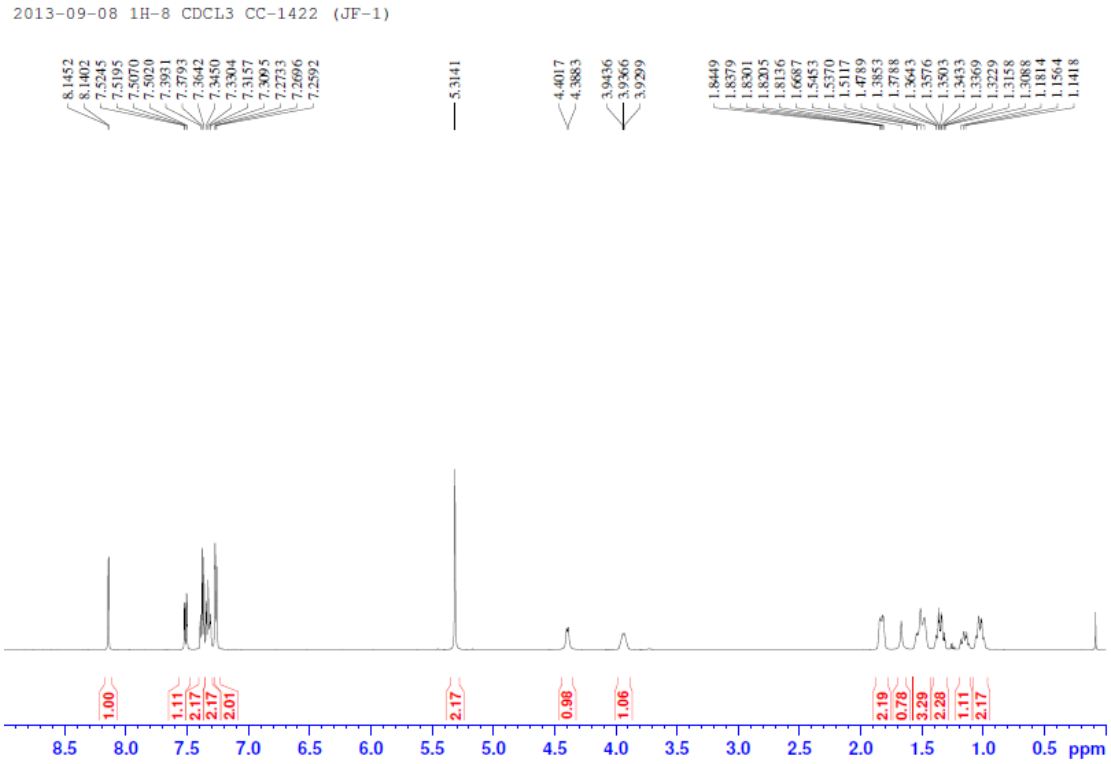

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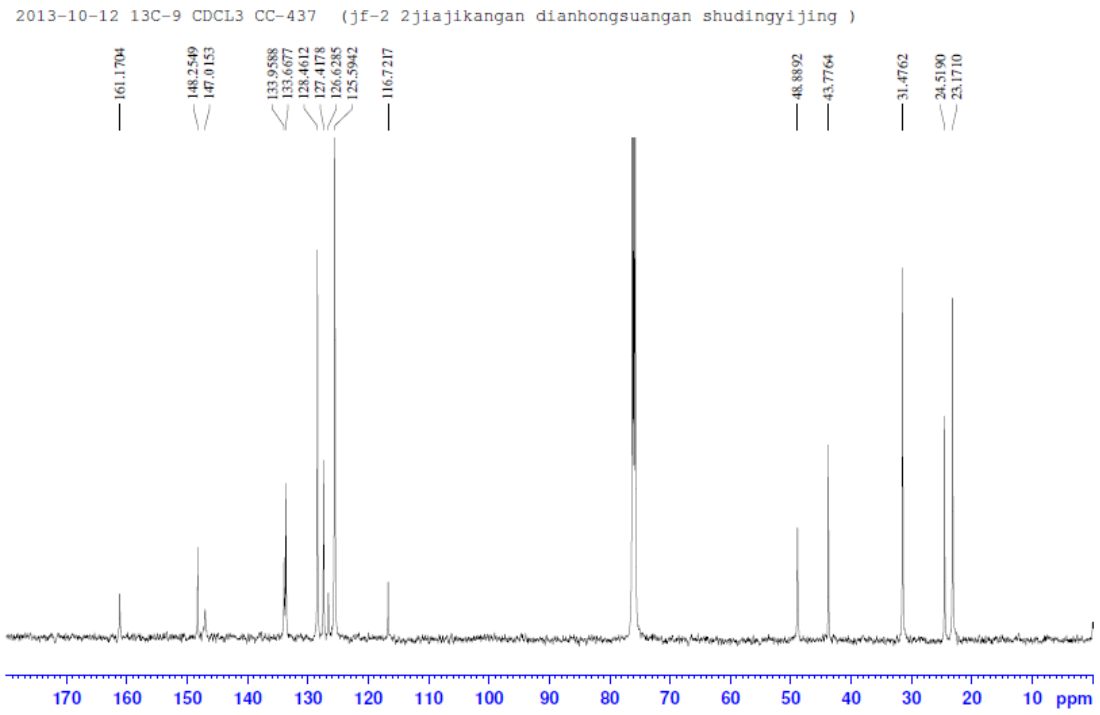

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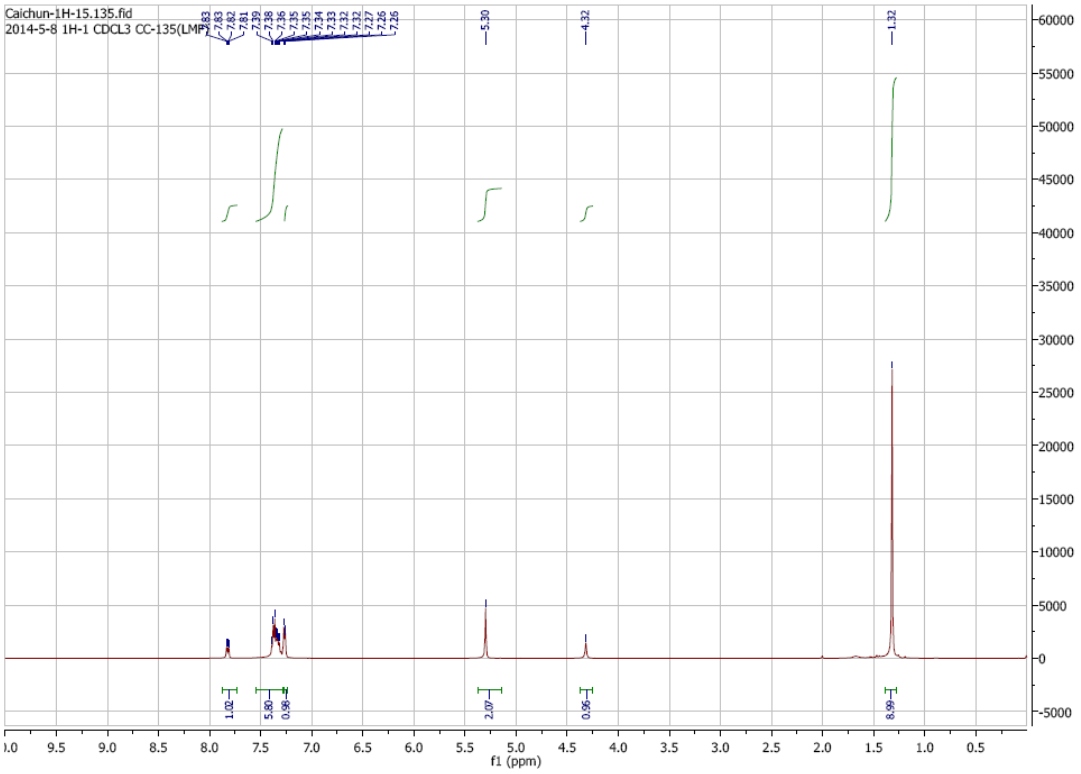

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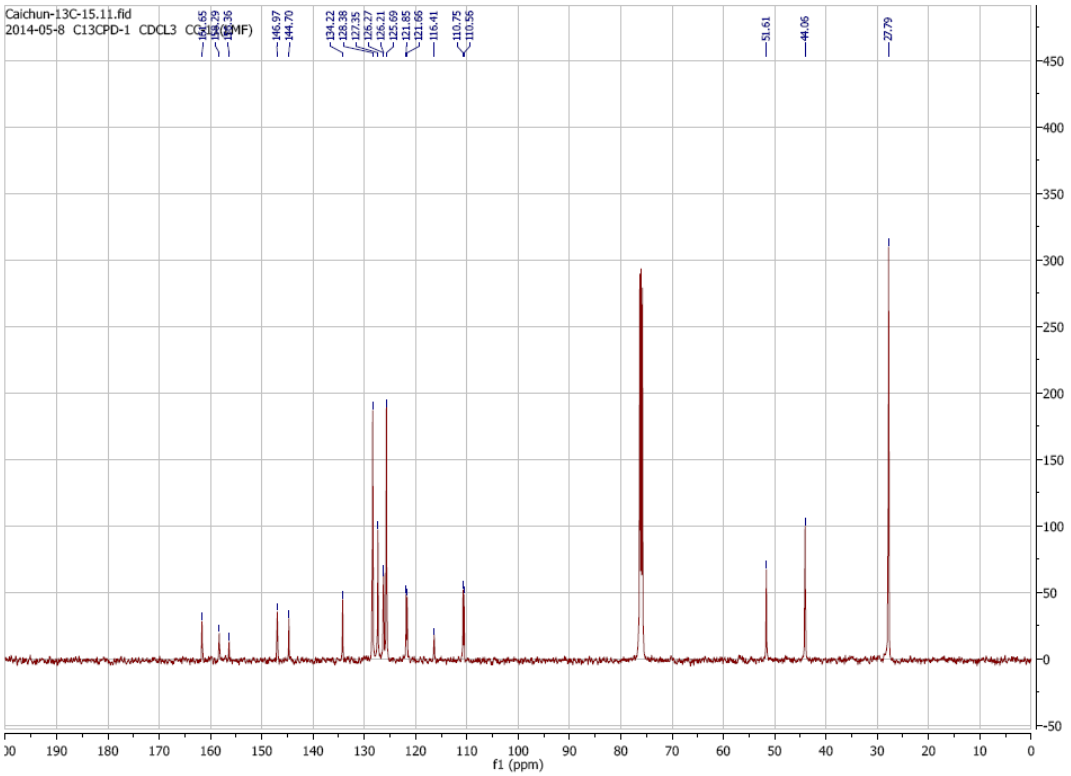

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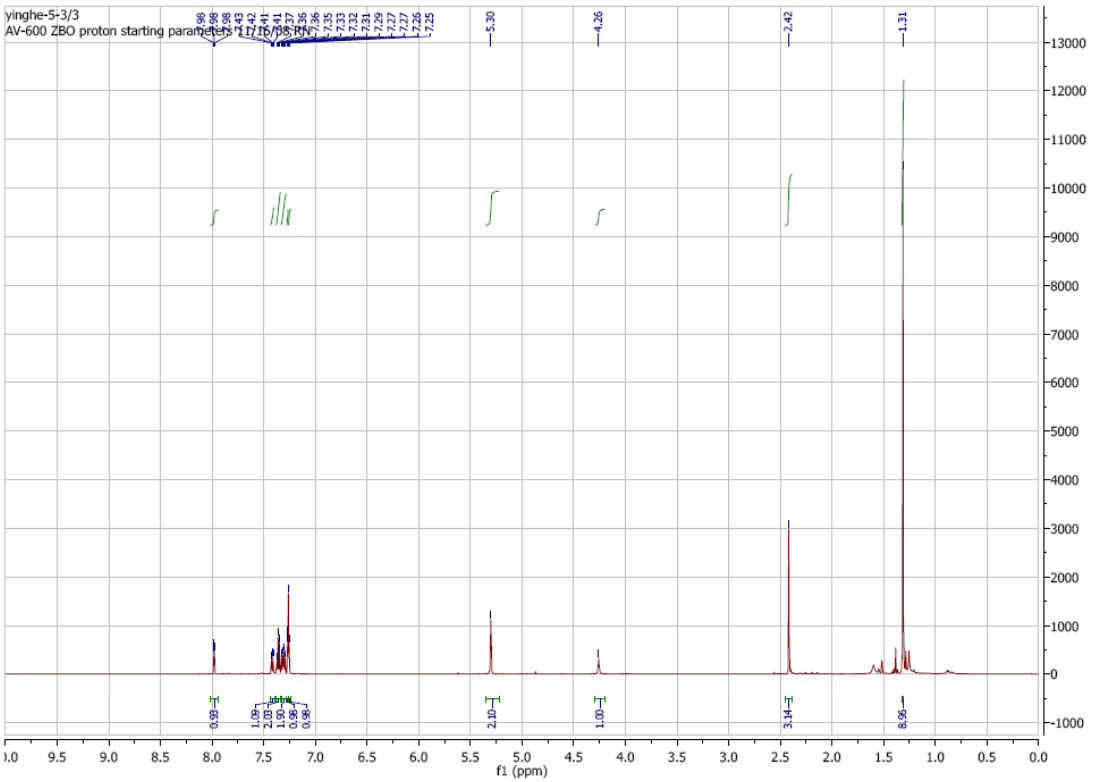

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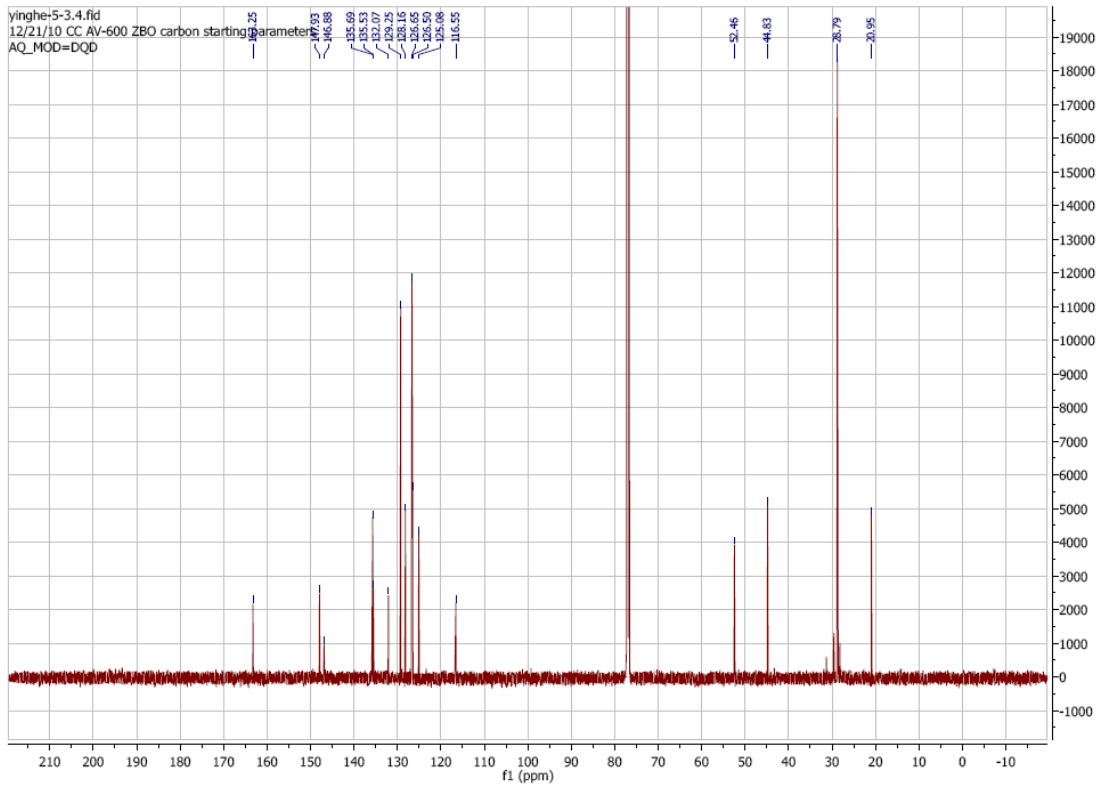

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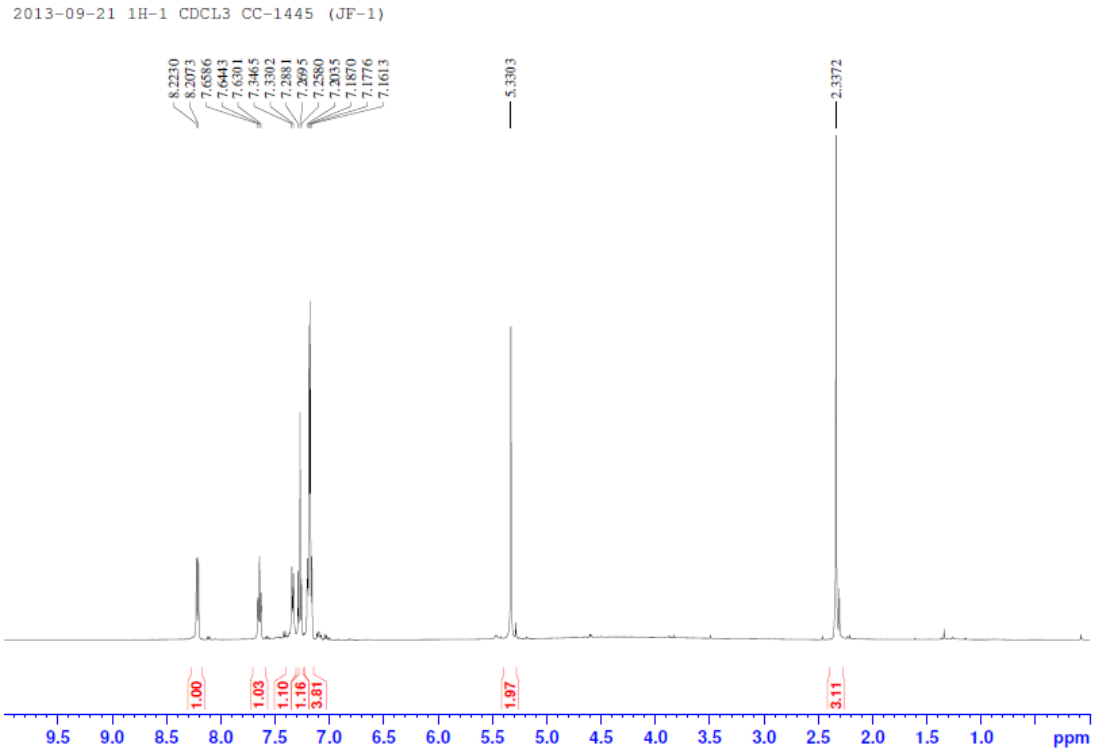

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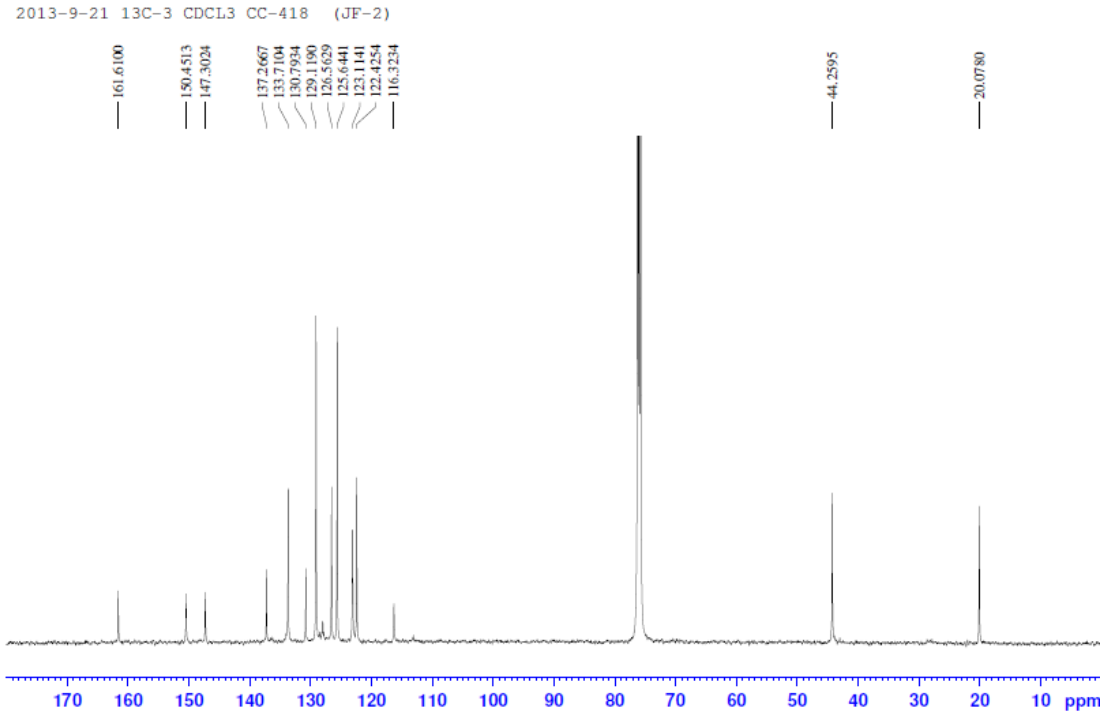

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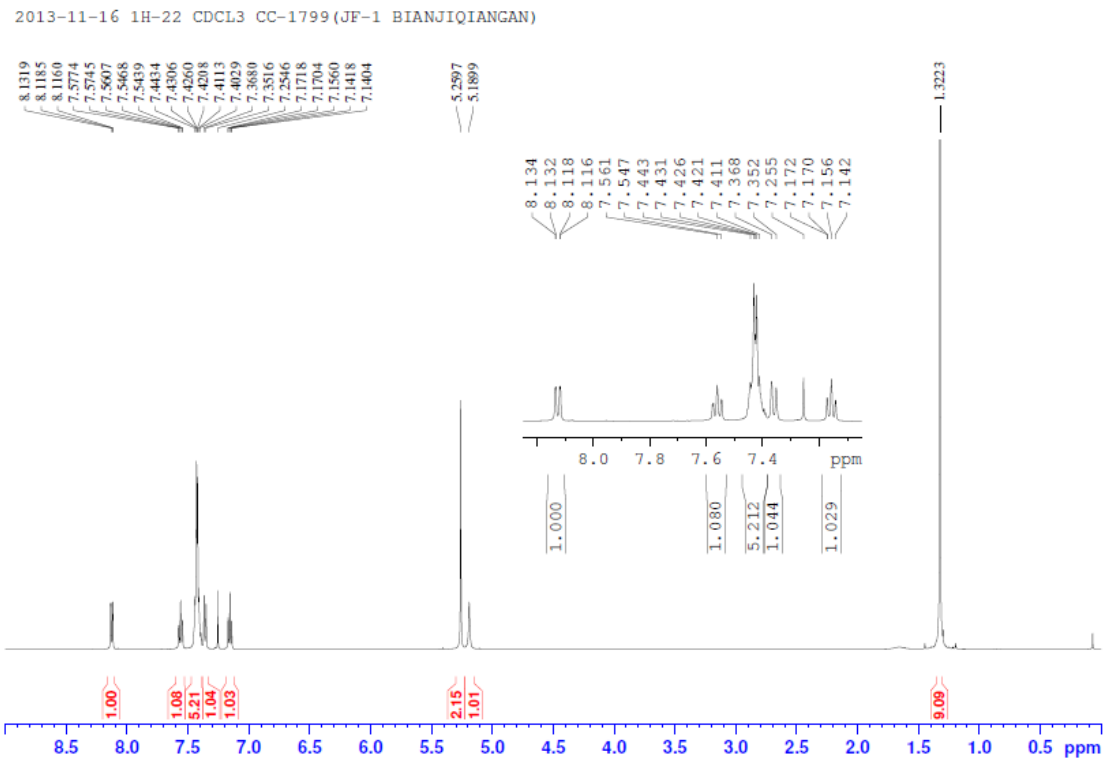

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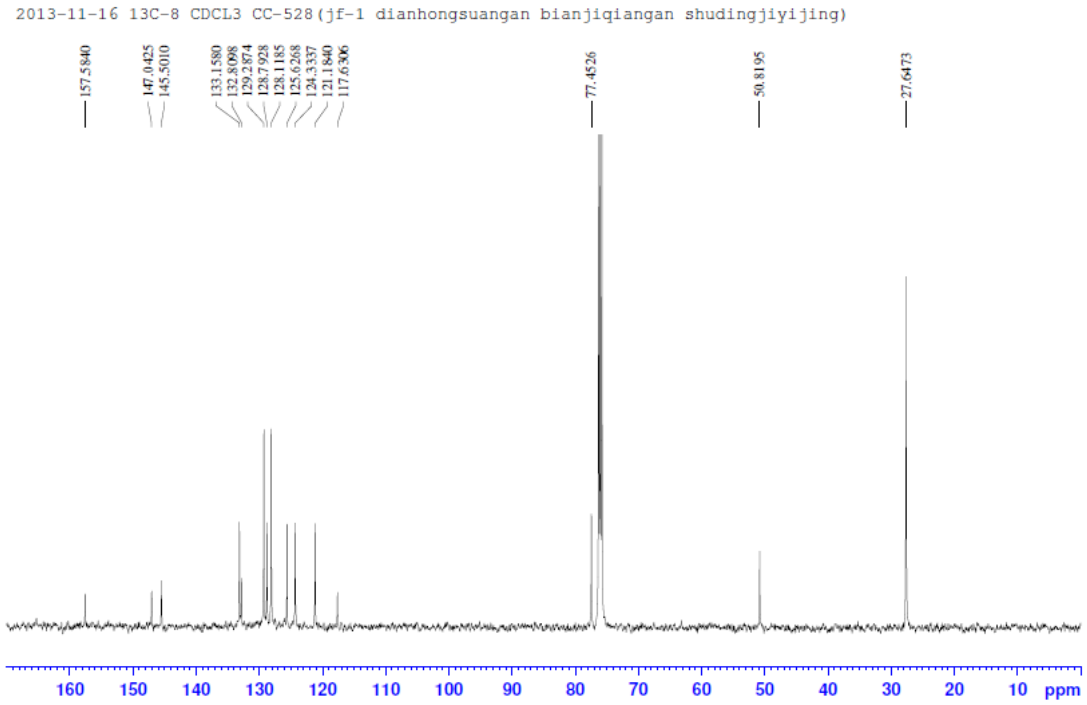

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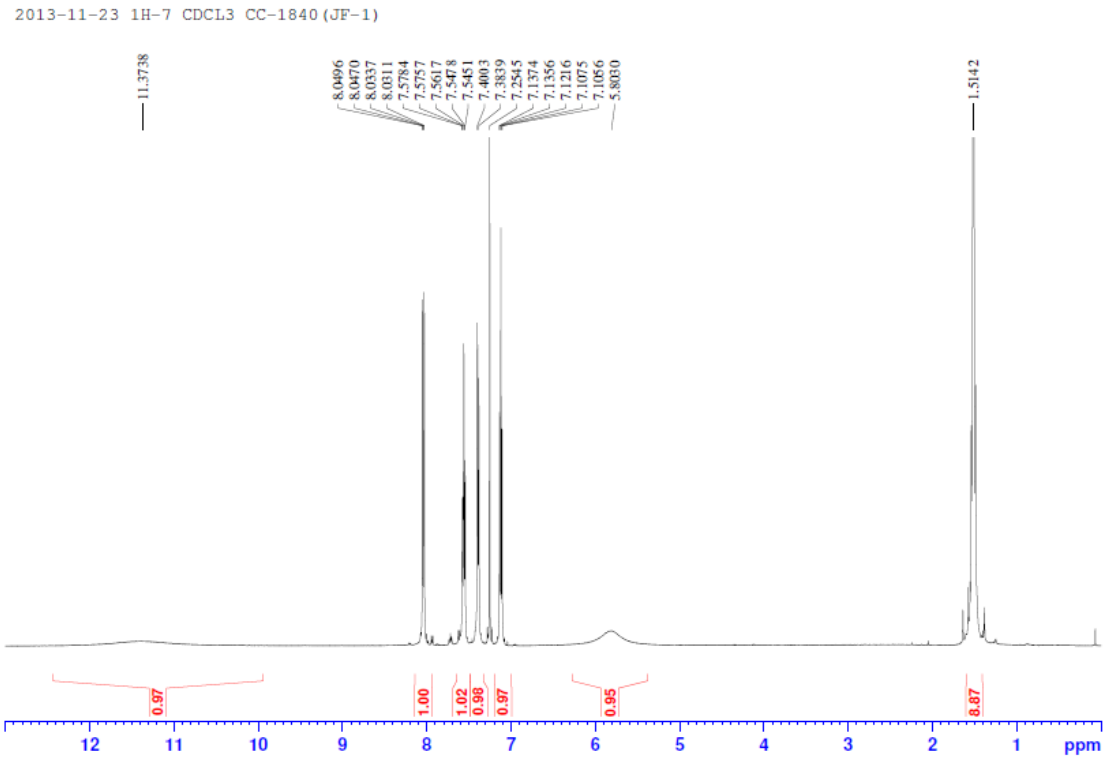

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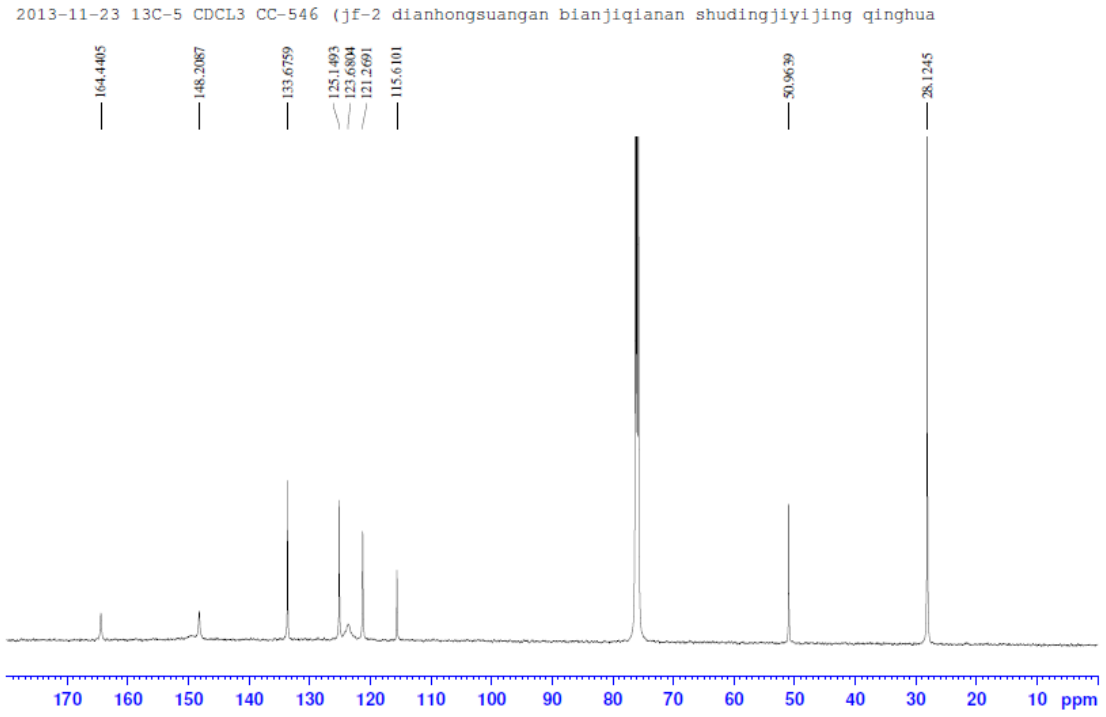
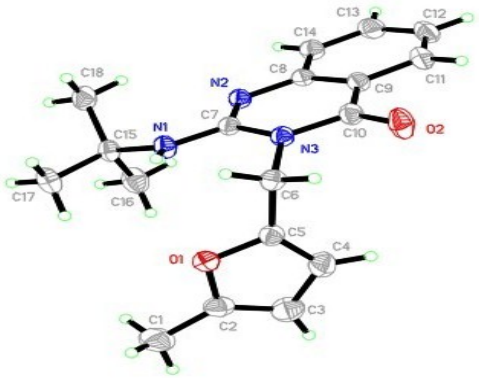


^{13}C NMR of compound **4w**

Single-crystal X-ray analysis of product 4j

Crystallographic data (excluding structure factors) for compound **4j** (CCDC 966928) have been deposited with the Cambridge Crystallographic Data Centre. Crystallographic data of complexes was collected at 296 K on a Bruker SMART CCD system equipped with graphite-monochromated Mo-Kα radiation (λ = 0.071073 nm) using ω-φ scan technique. Diffraction data were integrated by the SAINT program, which was also used for intensity corrections for Lorentz and polarization effects. Semi-empirical absorption correction was applied using SADABS. The structures were solved by direct methods and all non-hydrogen atoms were refined anisotropically on F^2 by full-matrix least-squares using the SHELXL-97 crystallographic software package.

complex	**4j**
Formula	$C_{18}H_{21}N_3O_2$
Formula weight	311.38
Crystal system	Monoclinic
space group	P2(1)/n
a (Å)	12.3807(10)
b (Å)	10.2922(8)
c (Å)	13.3591(10)
α (º)	90.00
β (º)	102.8390(10)
γ (º)	90.00
Volume($Å^3$)	1659.7(2)
Z	4
T, (K)	296(2)
D_{calcd} (g/m^3)	1.246
F(000)	664
Reflections collected	3094
Unique reflections	2409
Goof	1.028
R_1[I> 2σ(I)]	0.0412
wR_2[I>2σ(I)]	0.1086
CCDC number	CCDC 966928



Single-crystal X-ray analysis of **4j**