

Supporting Information

Beyond Acrylamide: A Structure-Guided Investigation of Covalent Warheads in the Development of CDK7 Inhibitors

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Contributed equally

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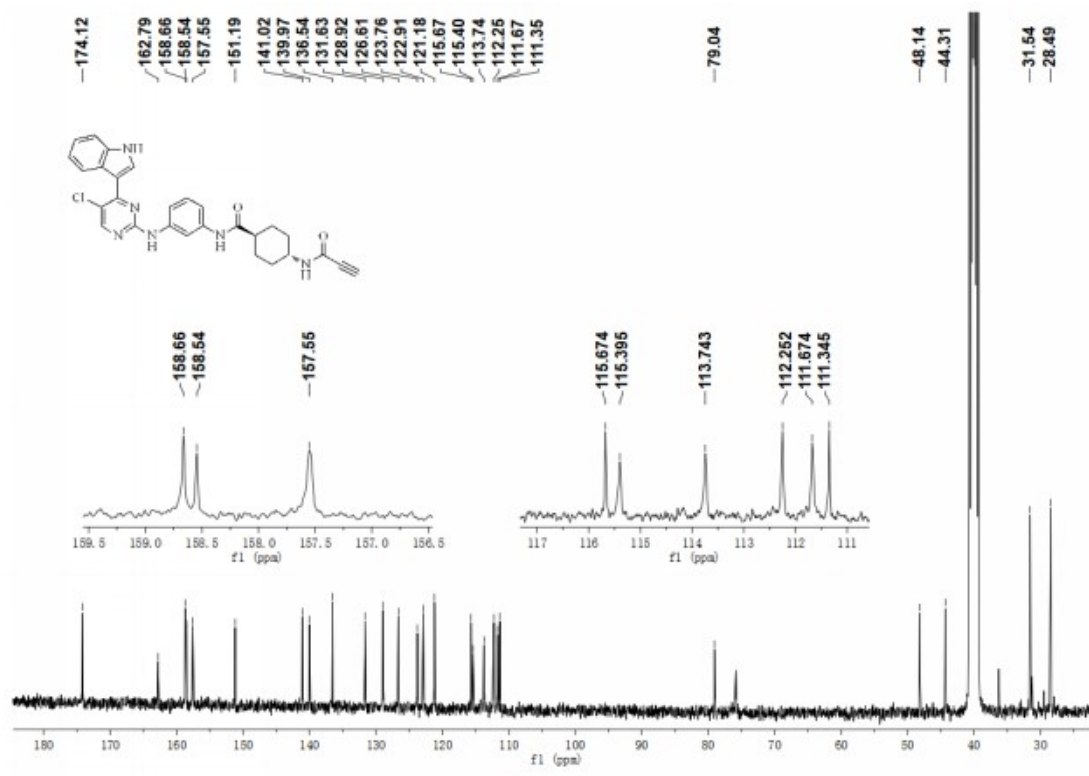
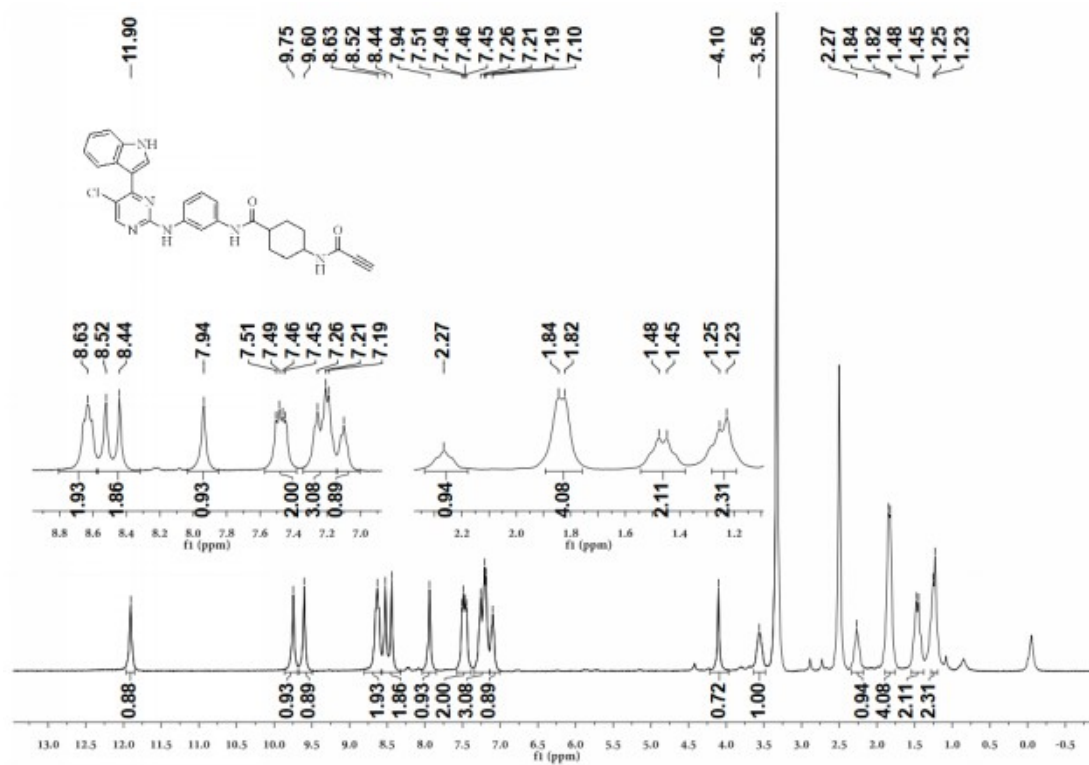
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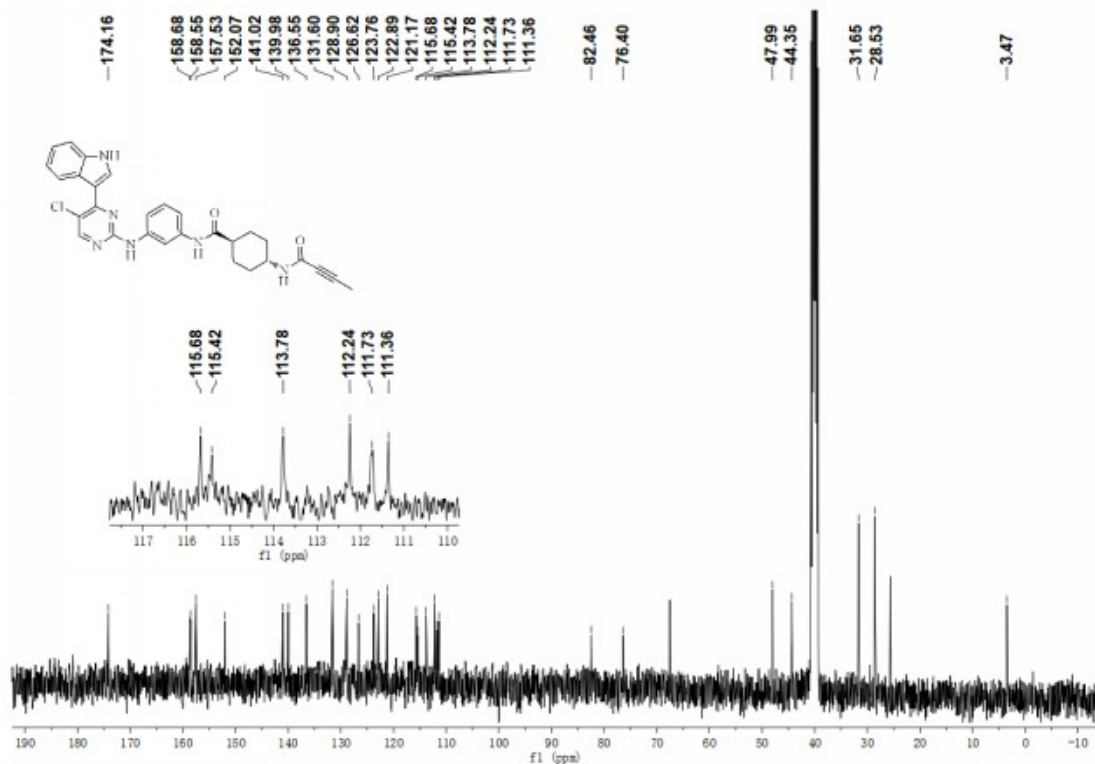
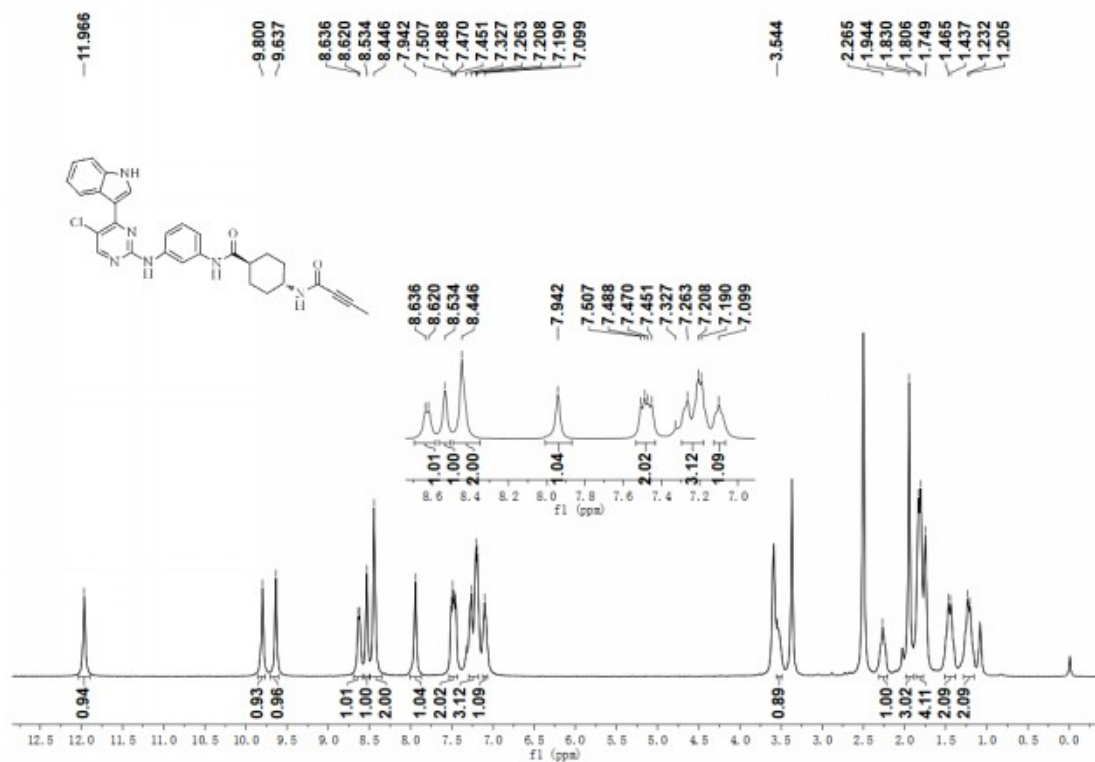
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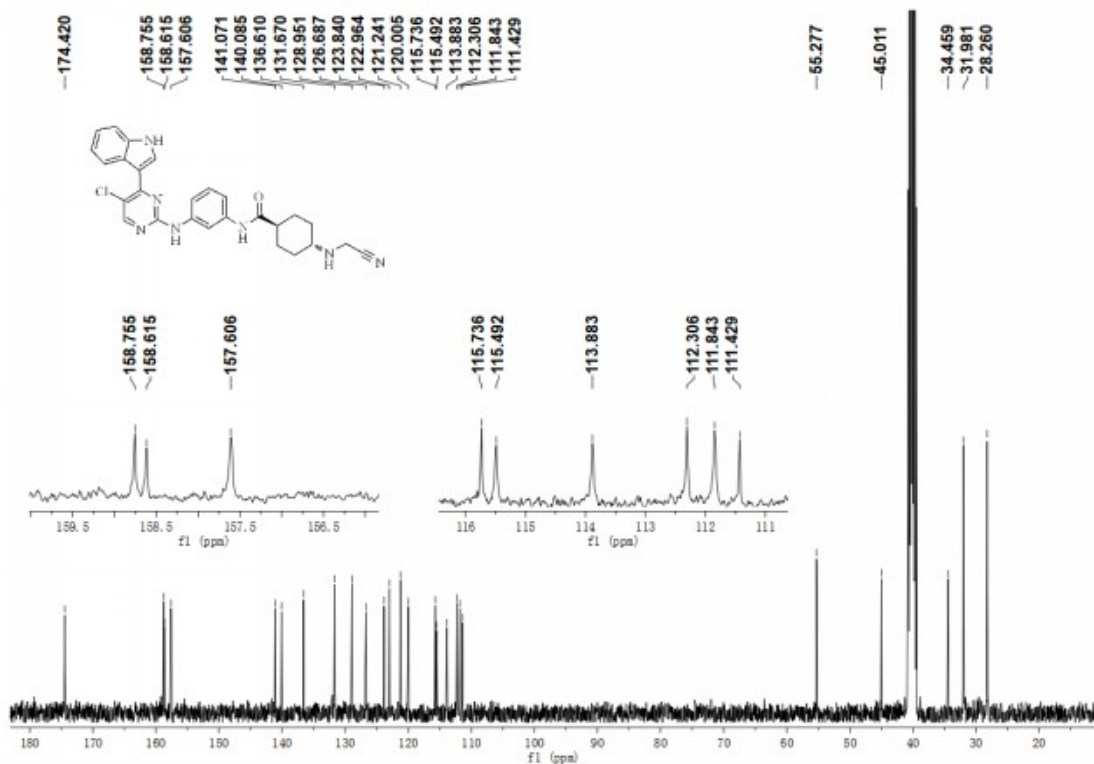
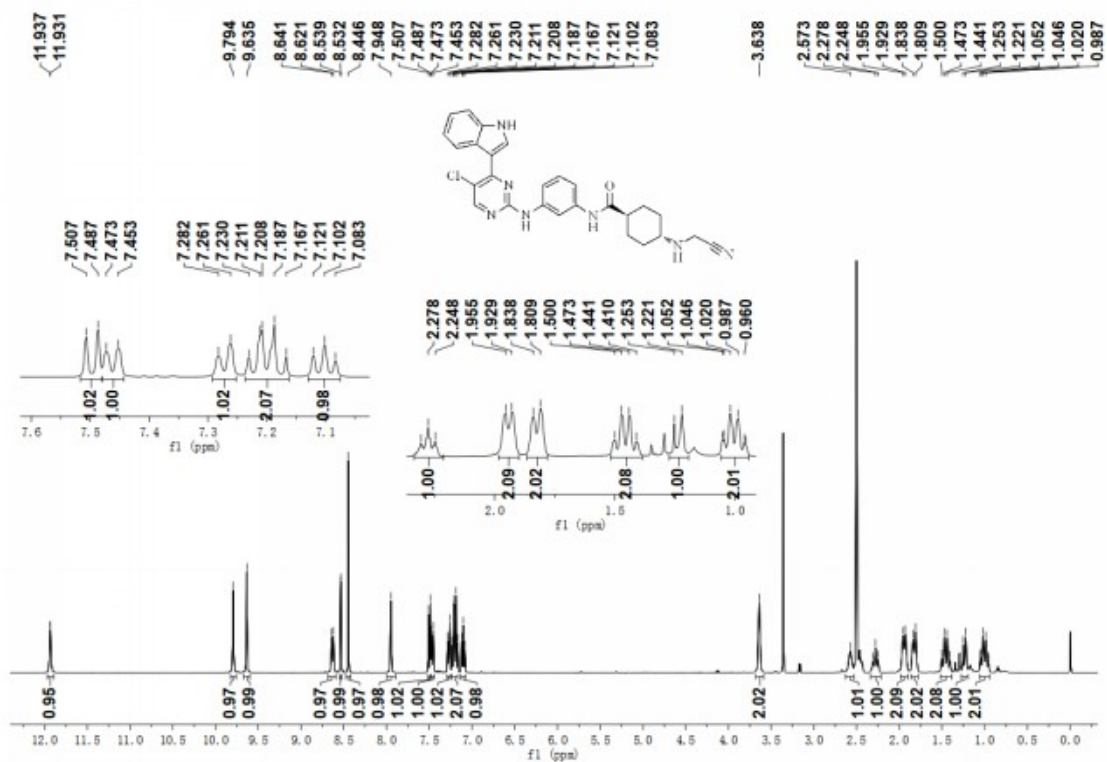
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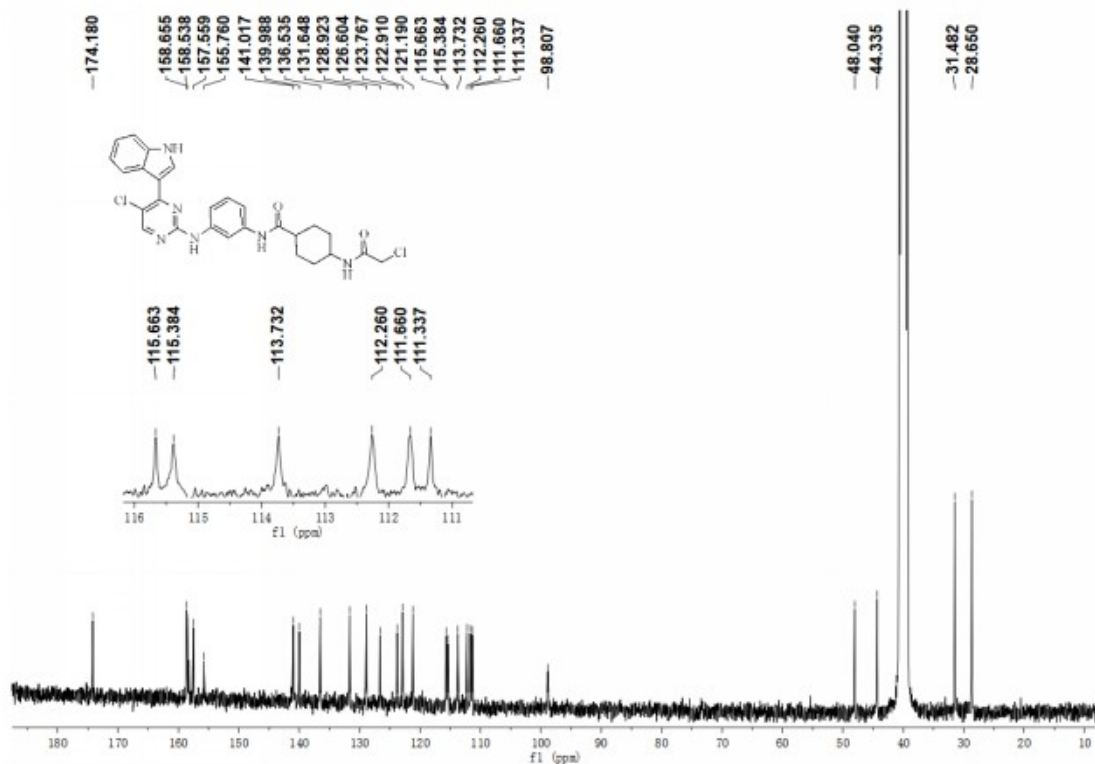
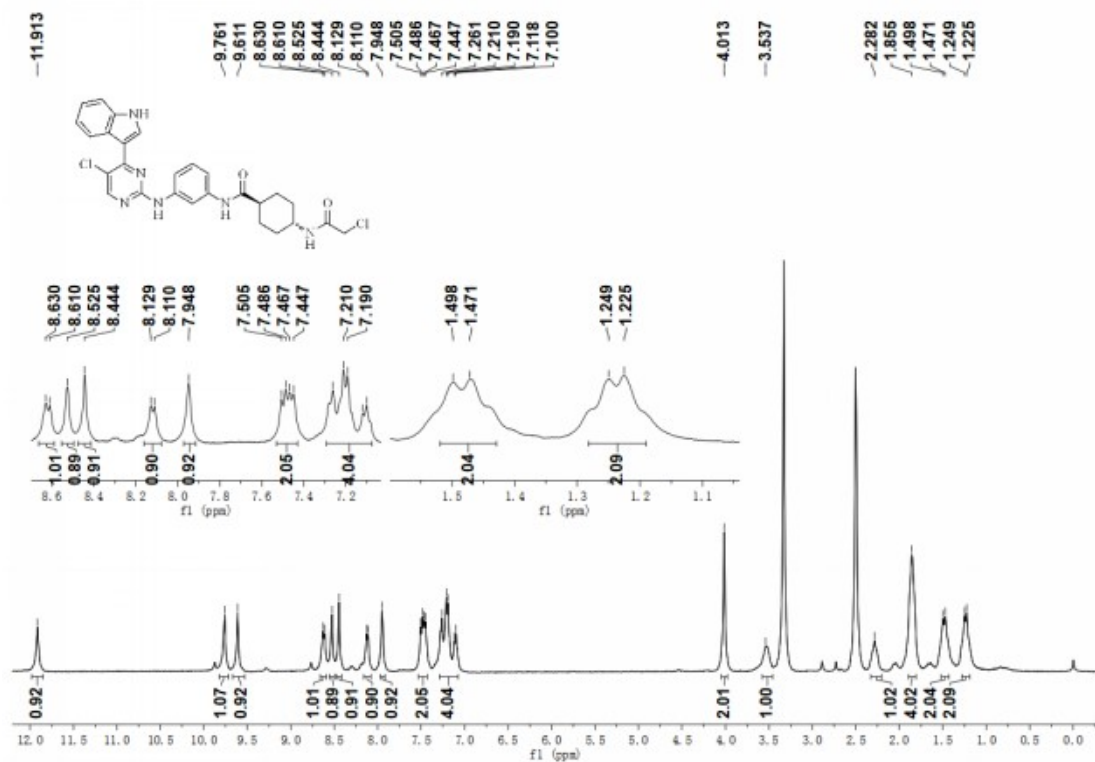
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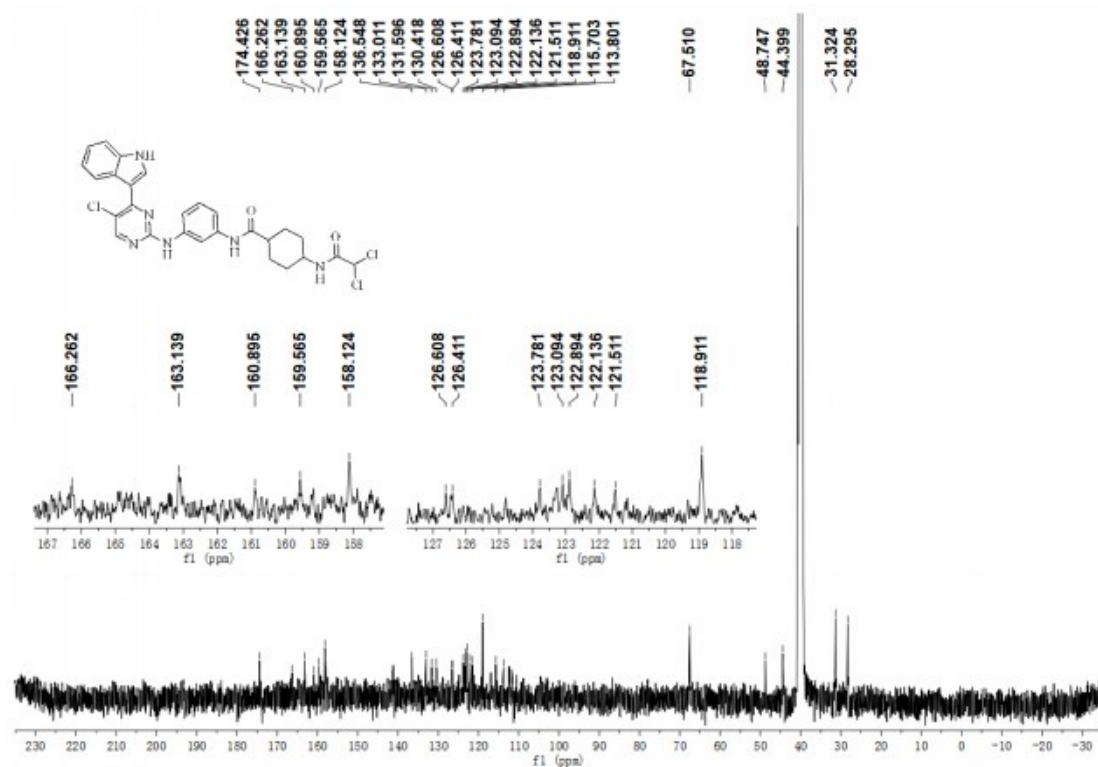
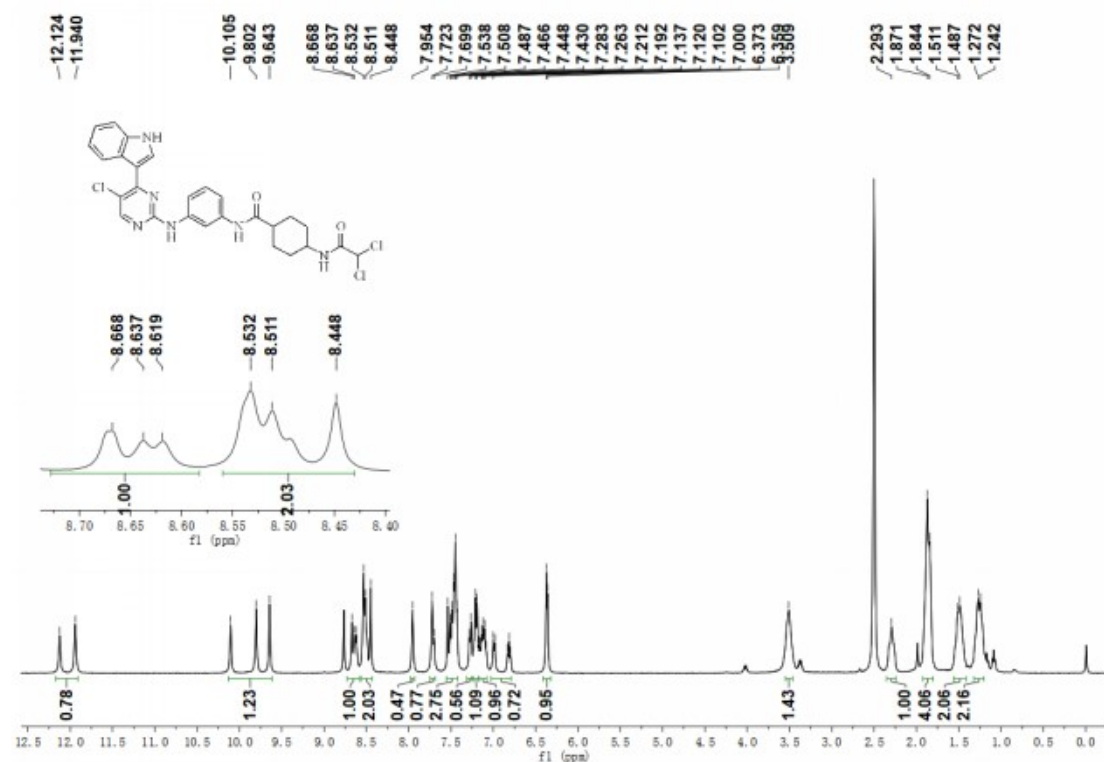
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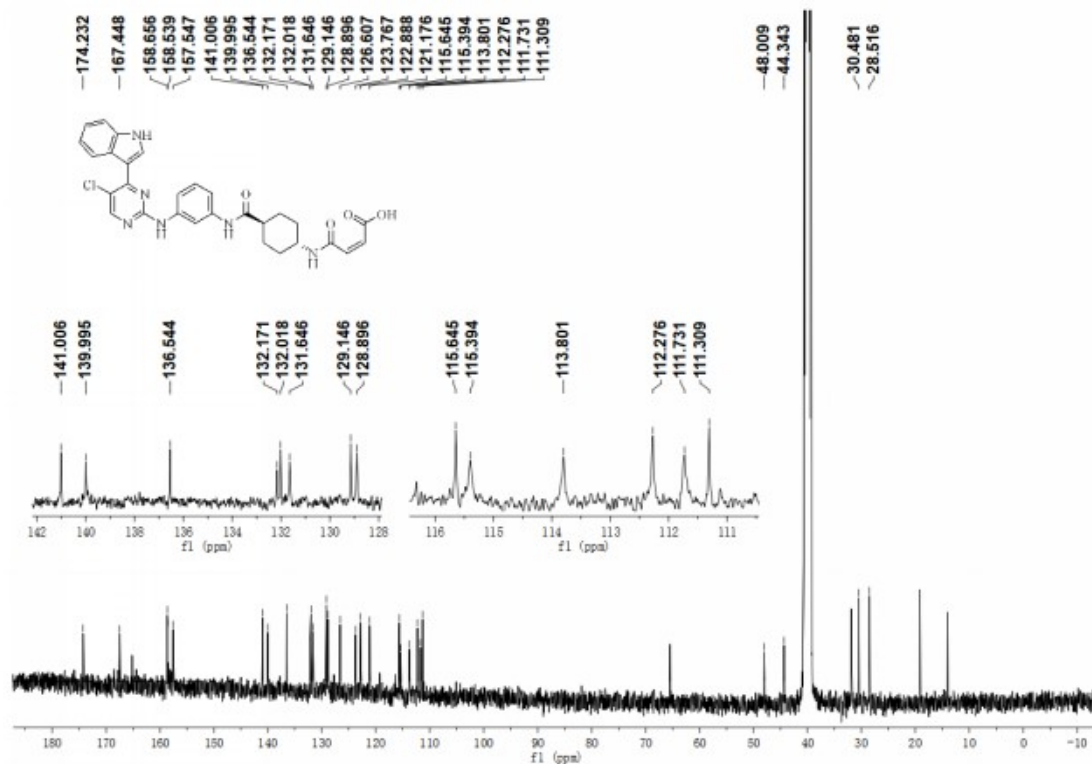
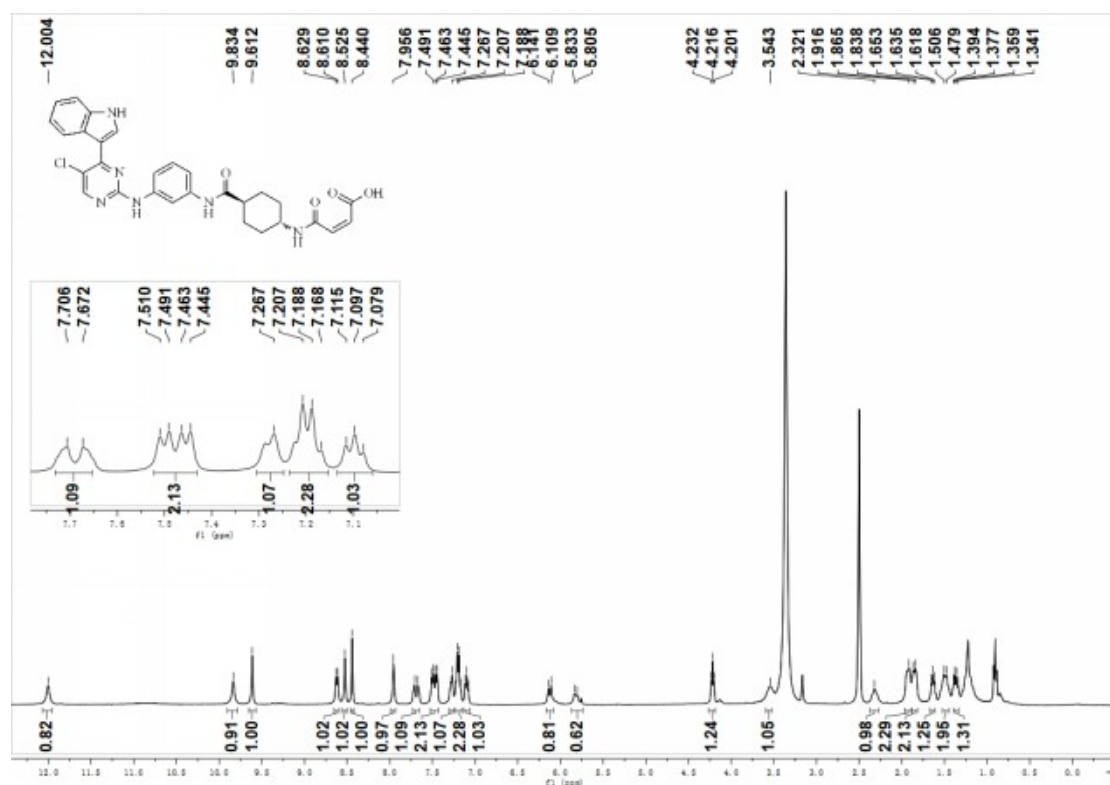
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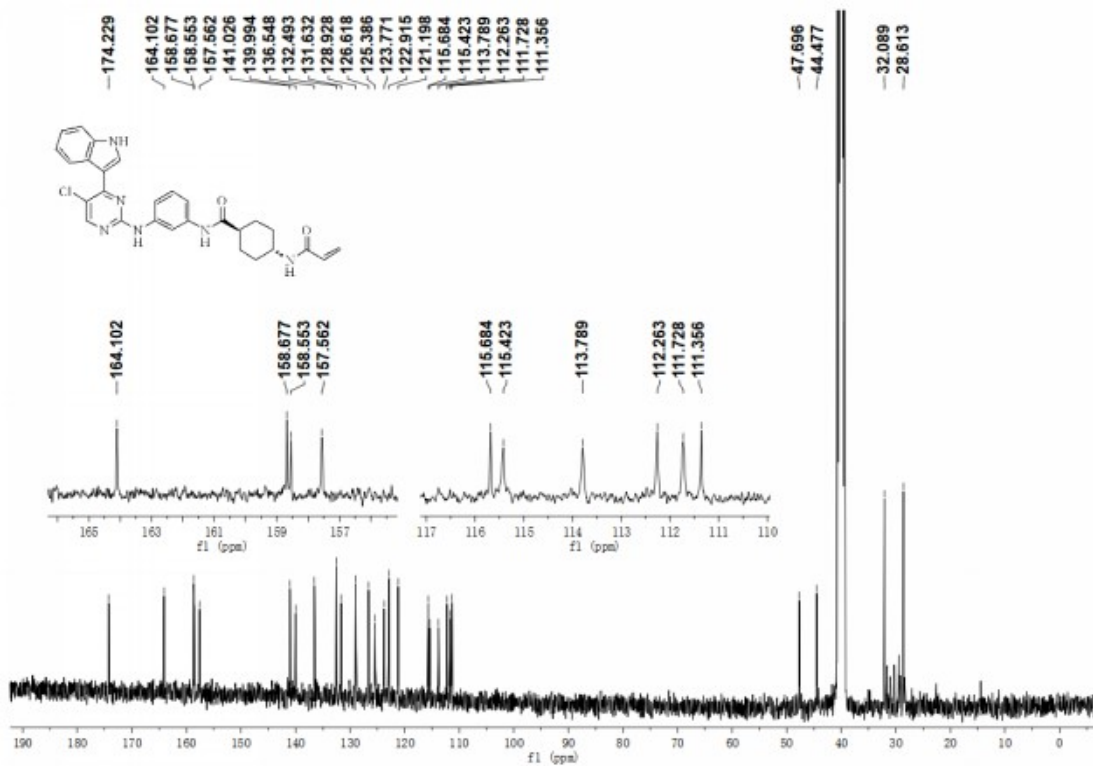
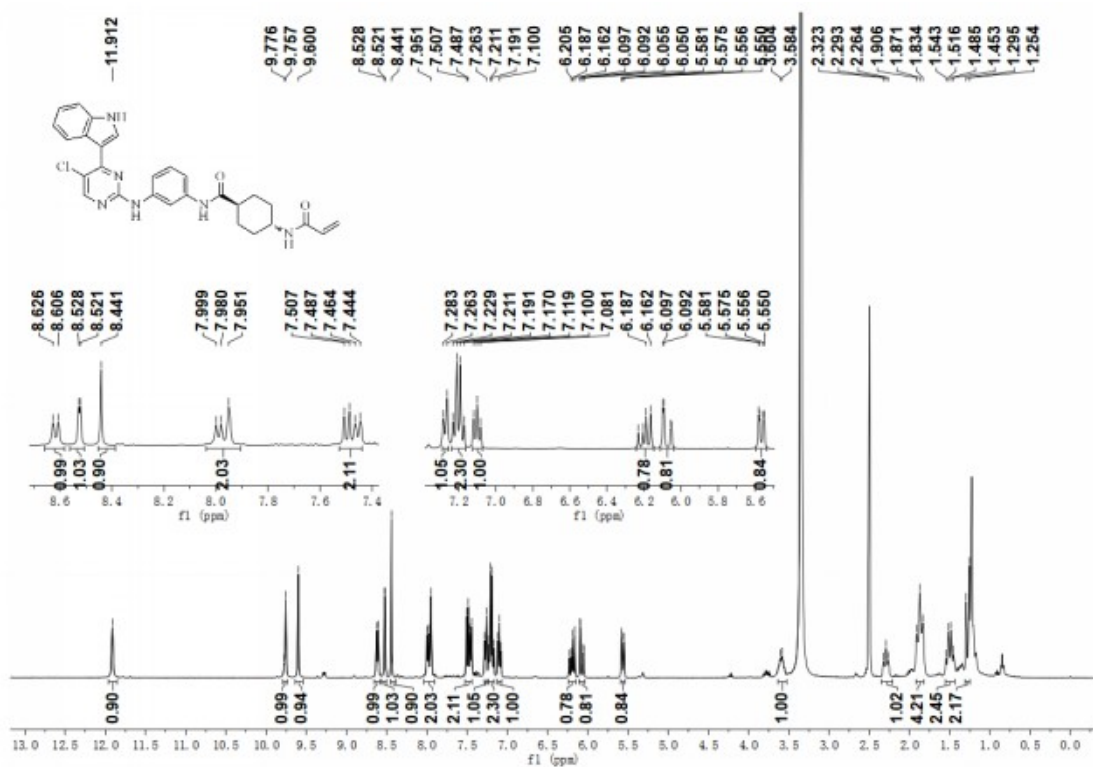
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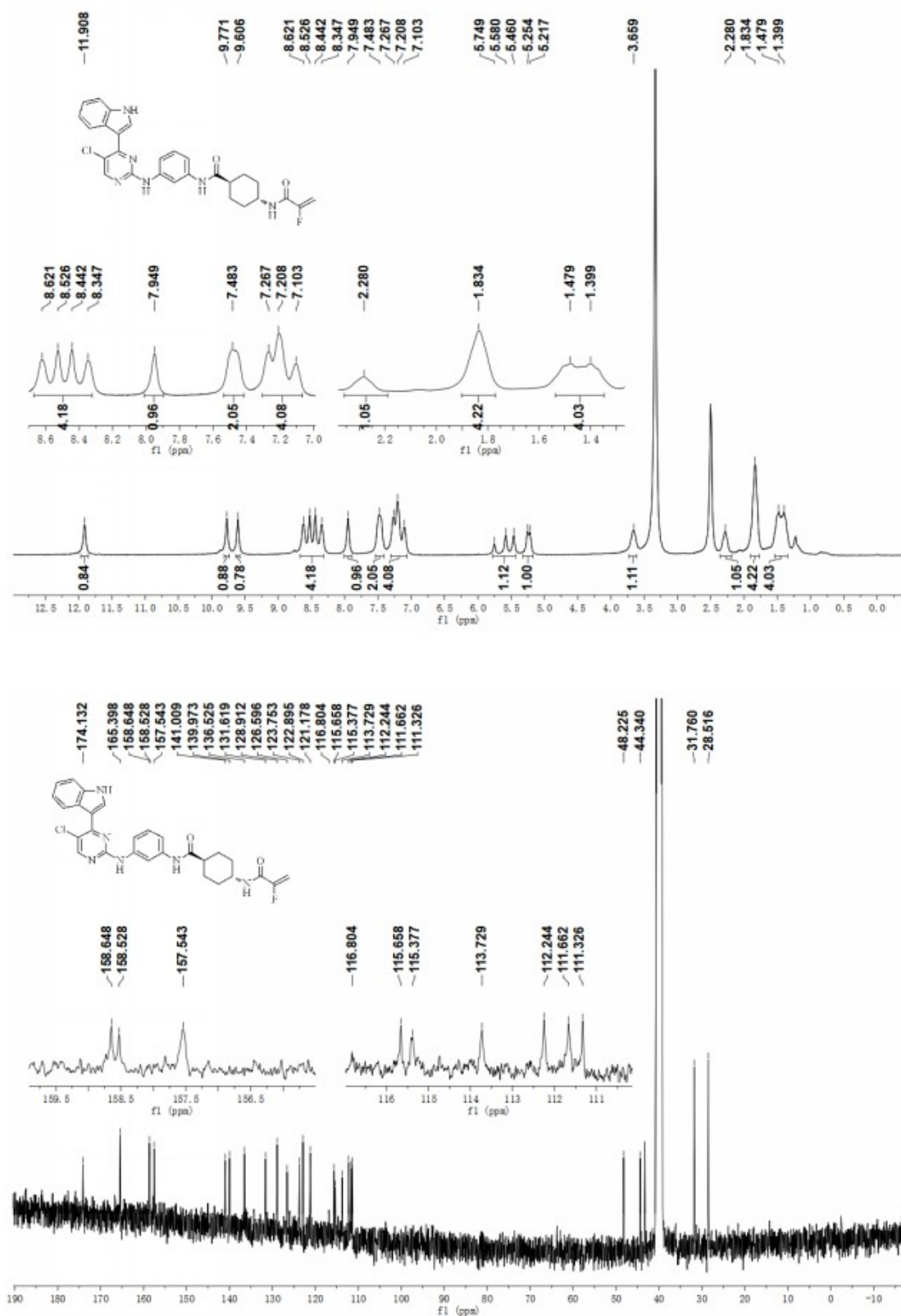
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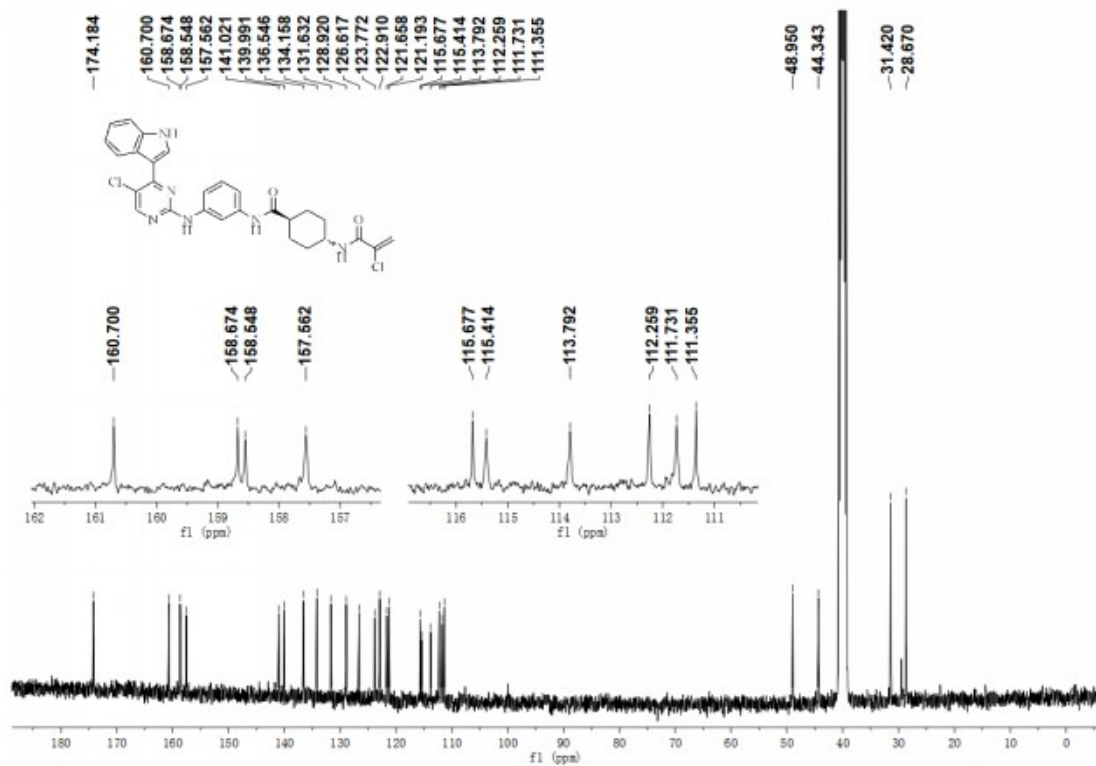
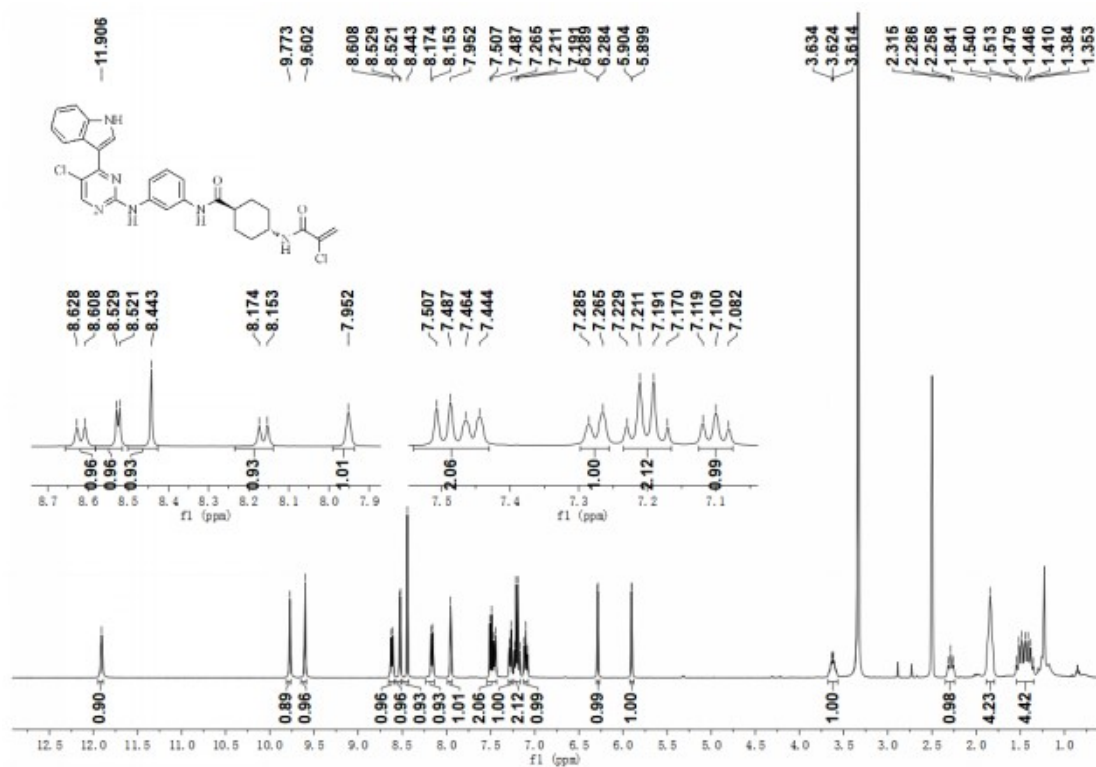
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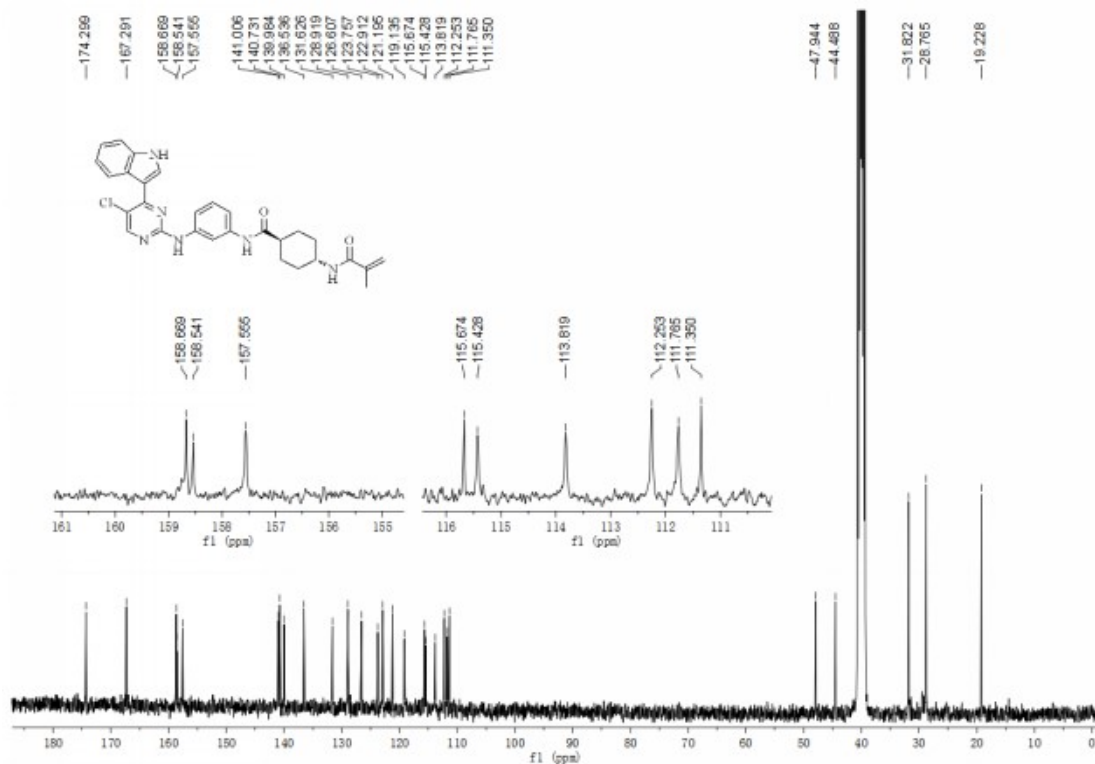
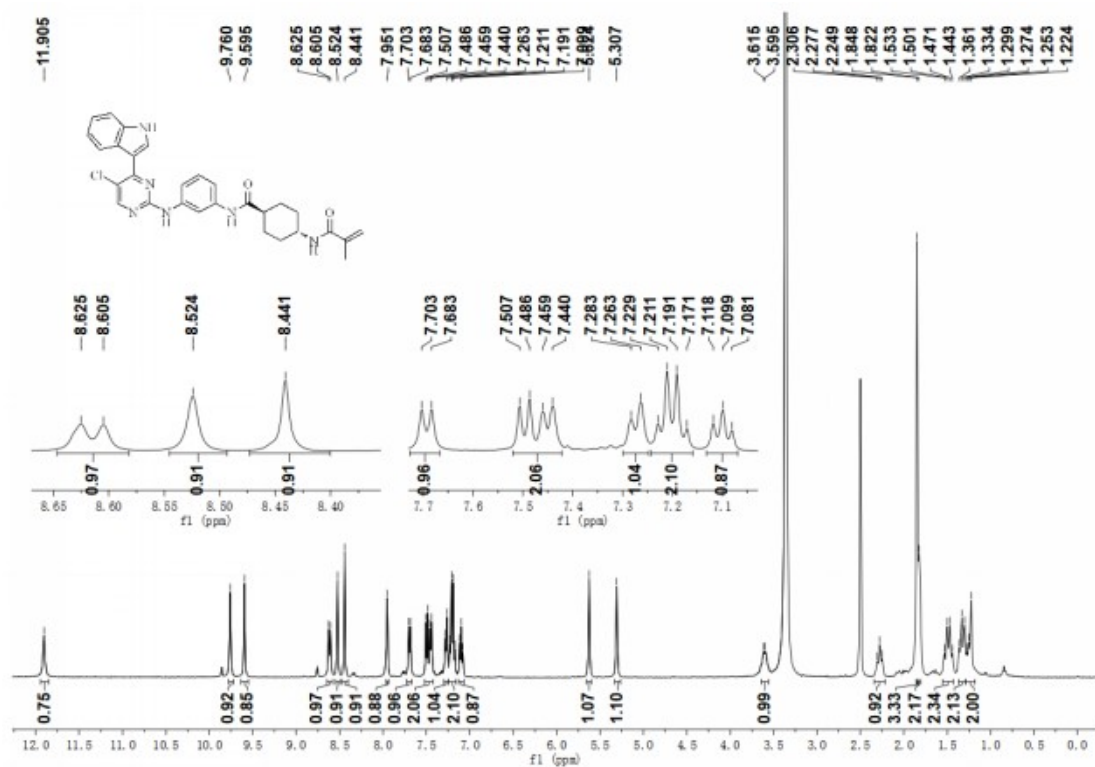
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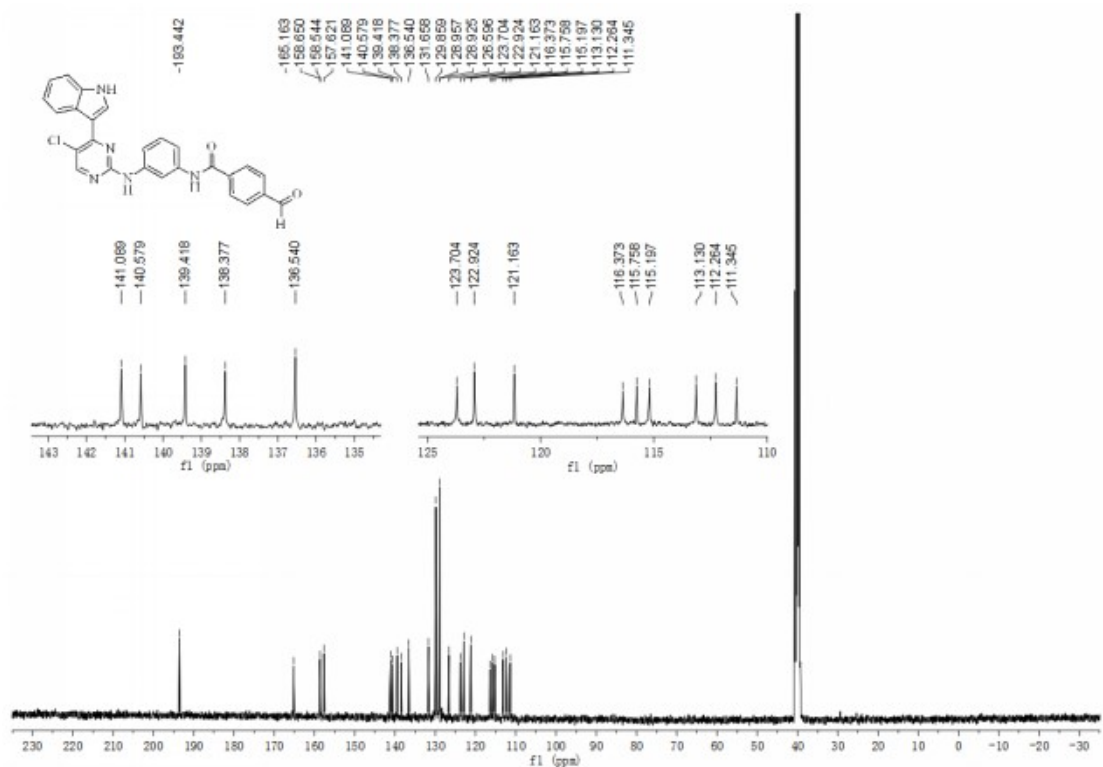
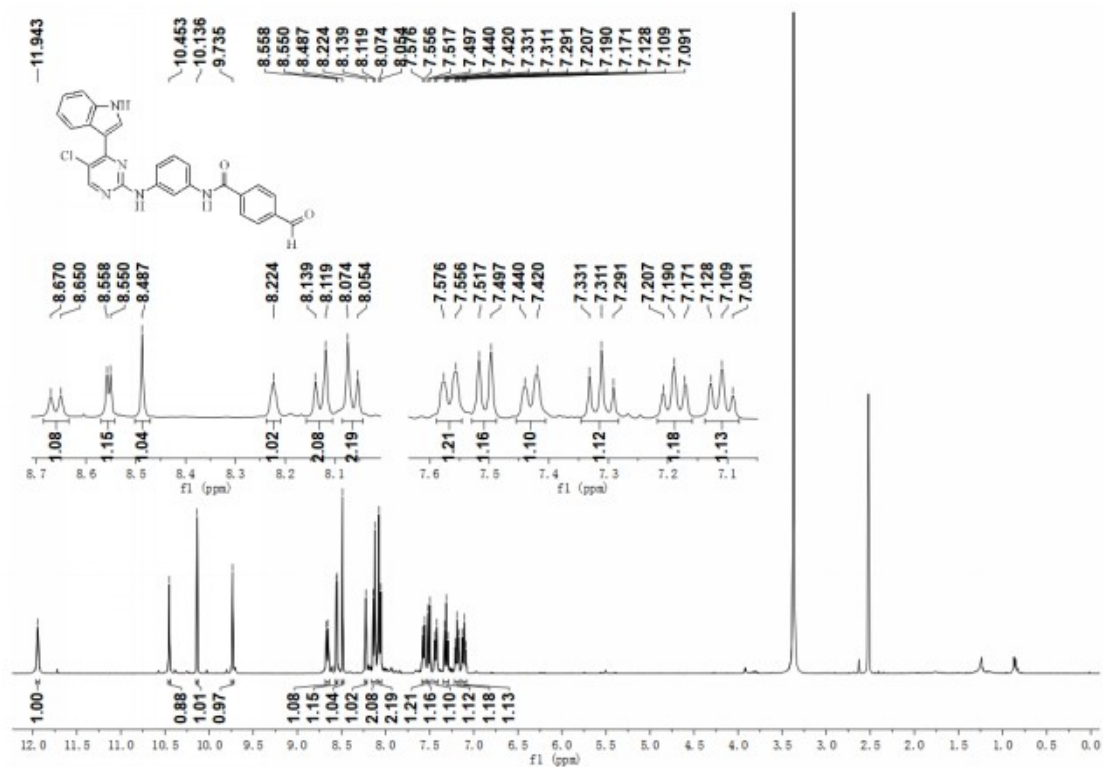
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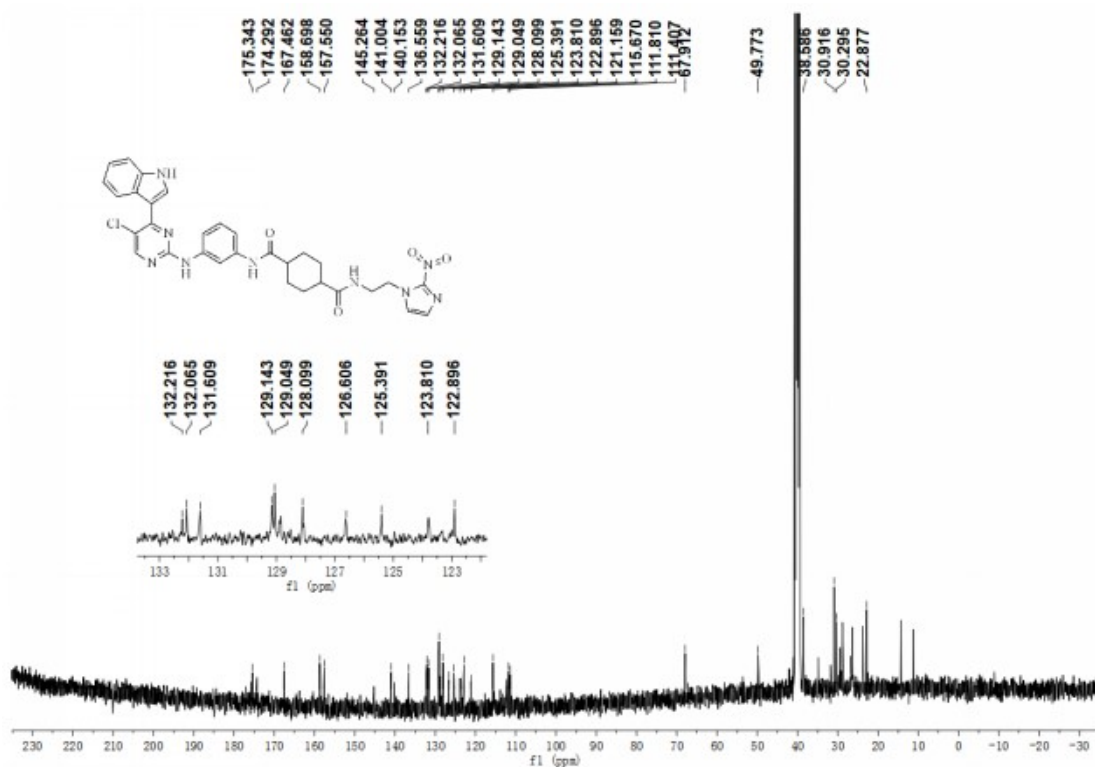
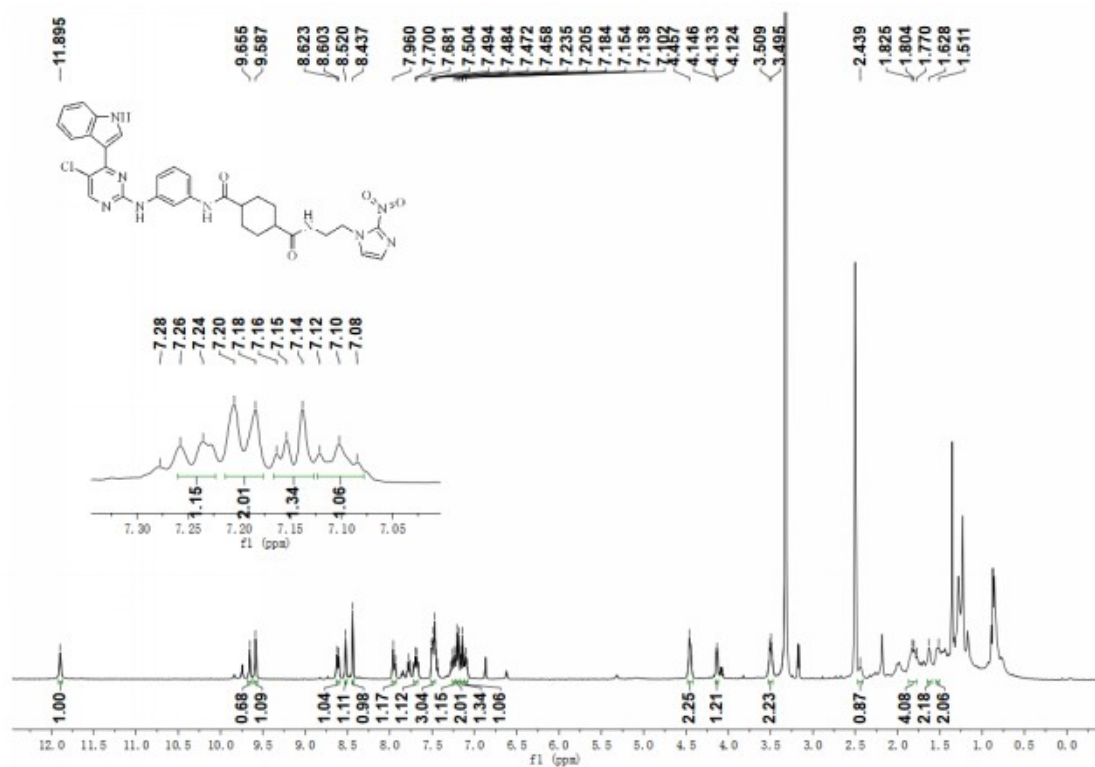
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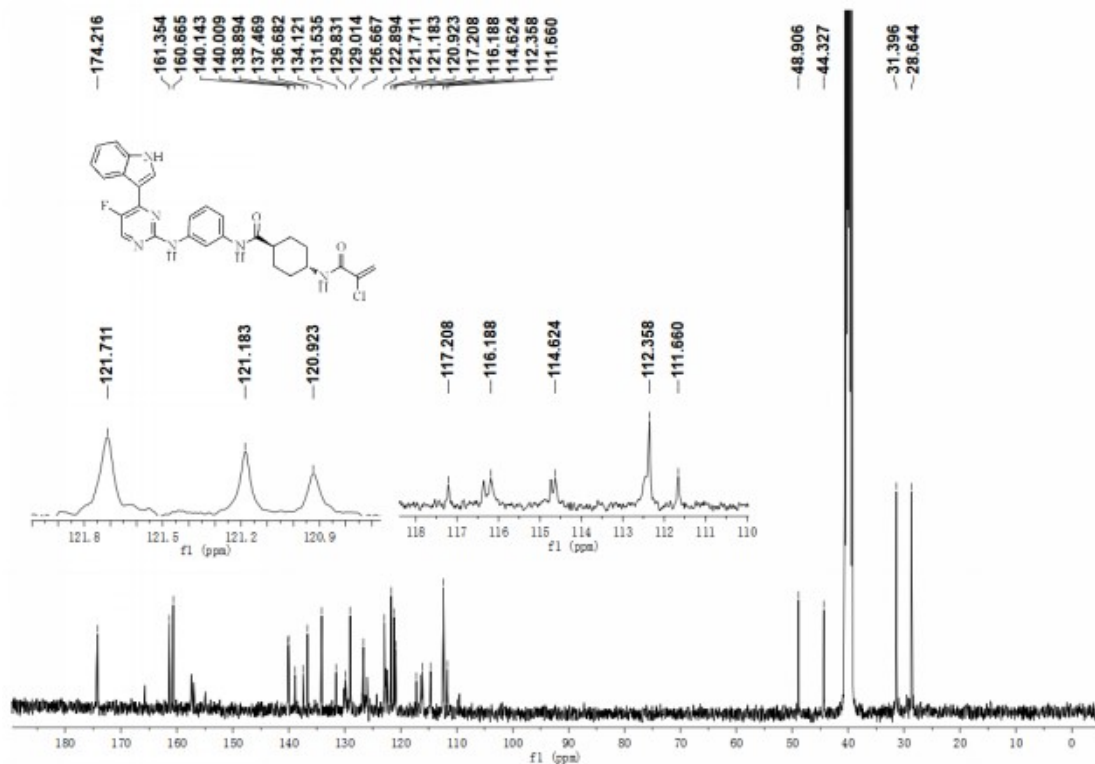
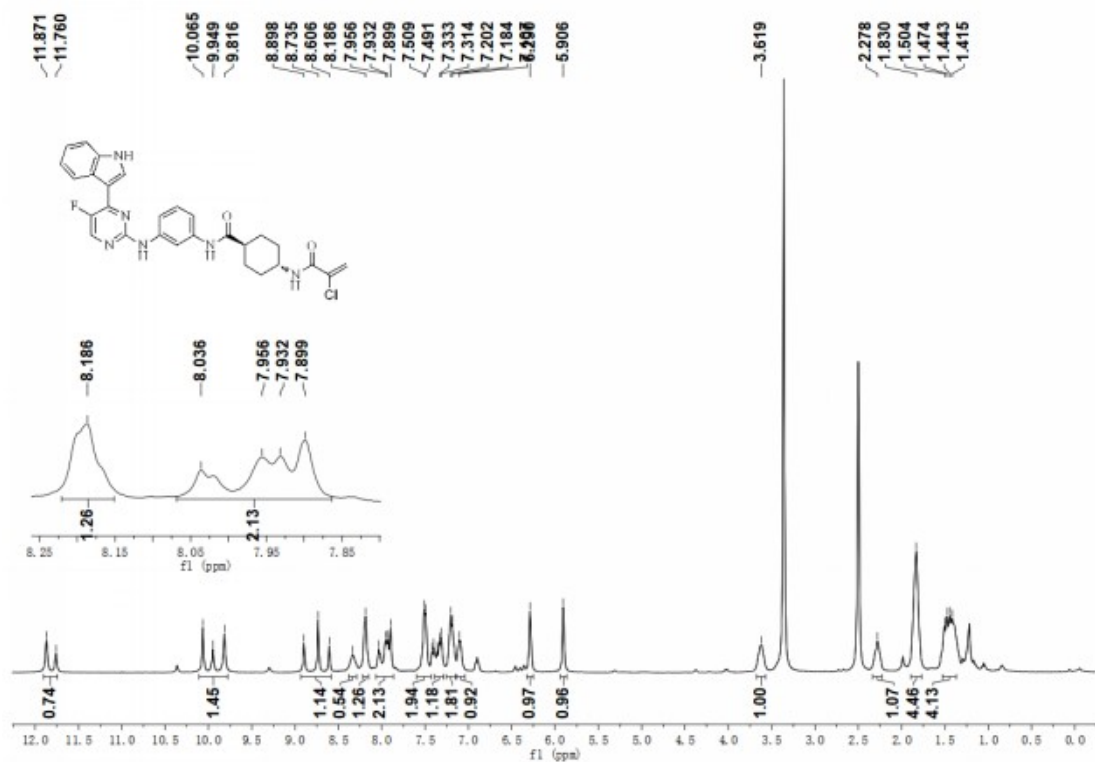
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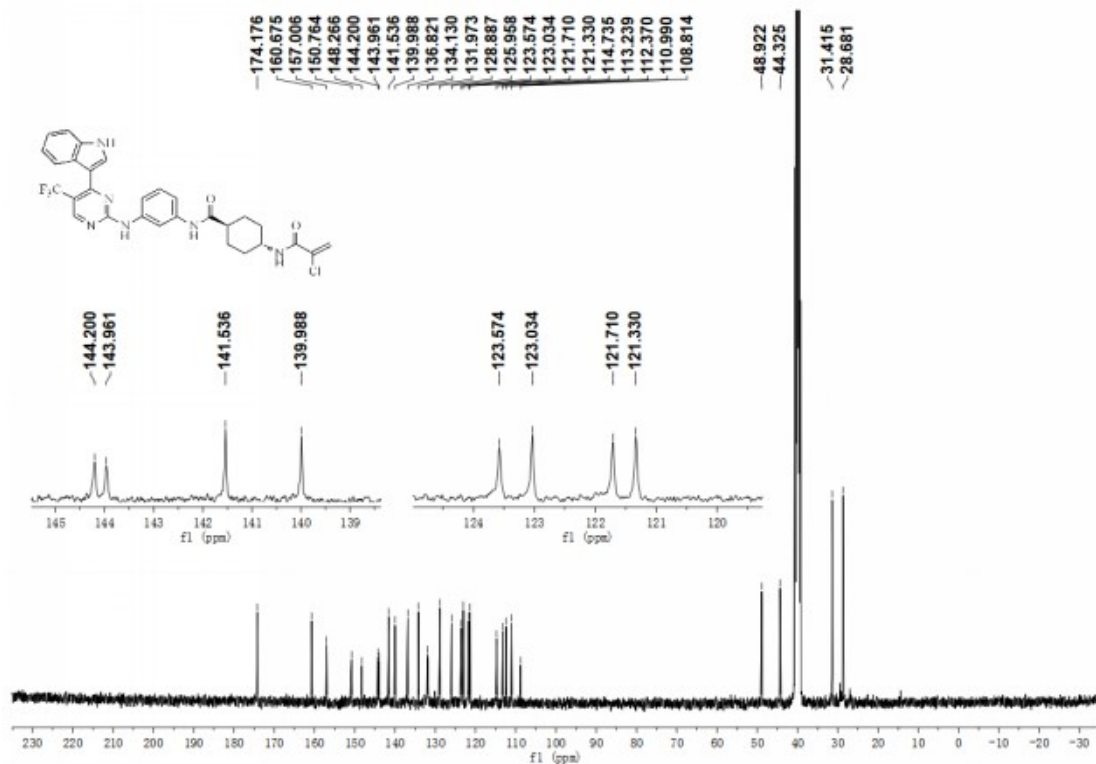
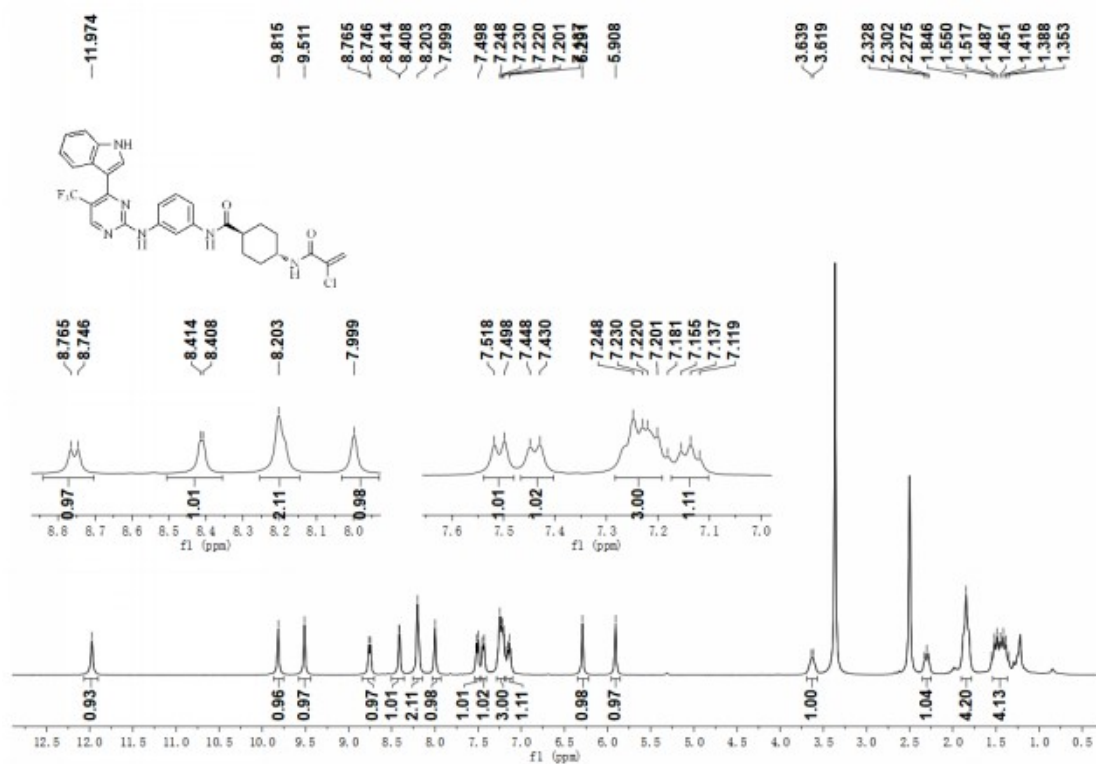
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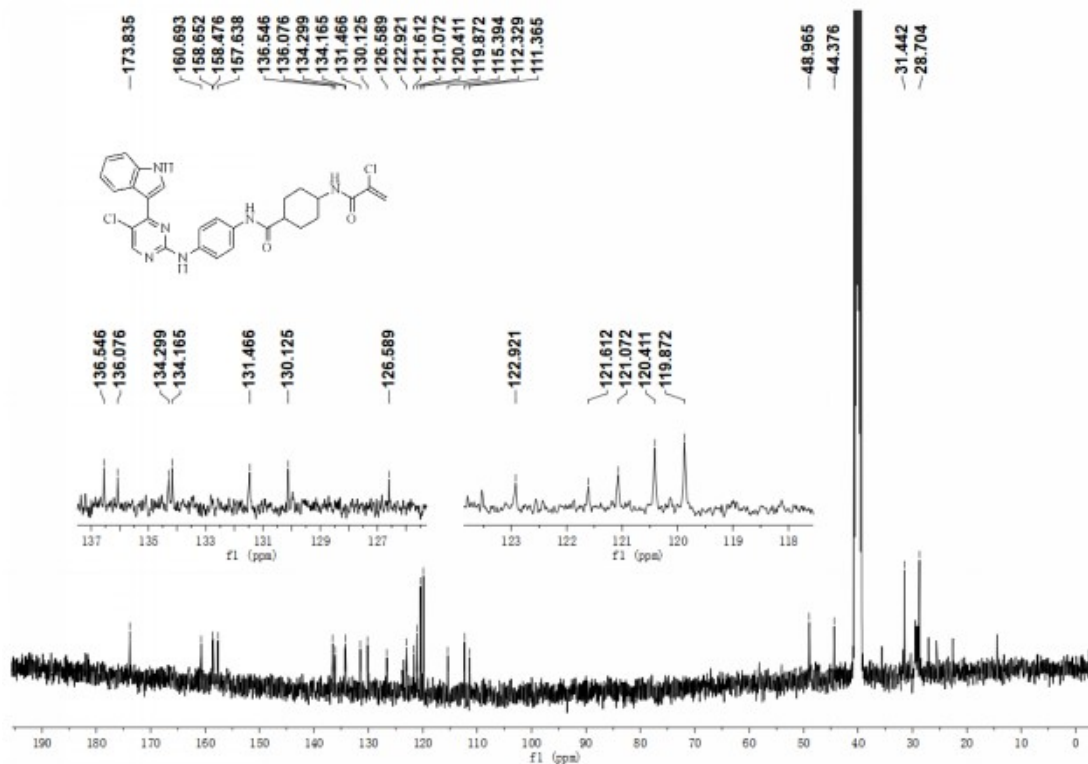
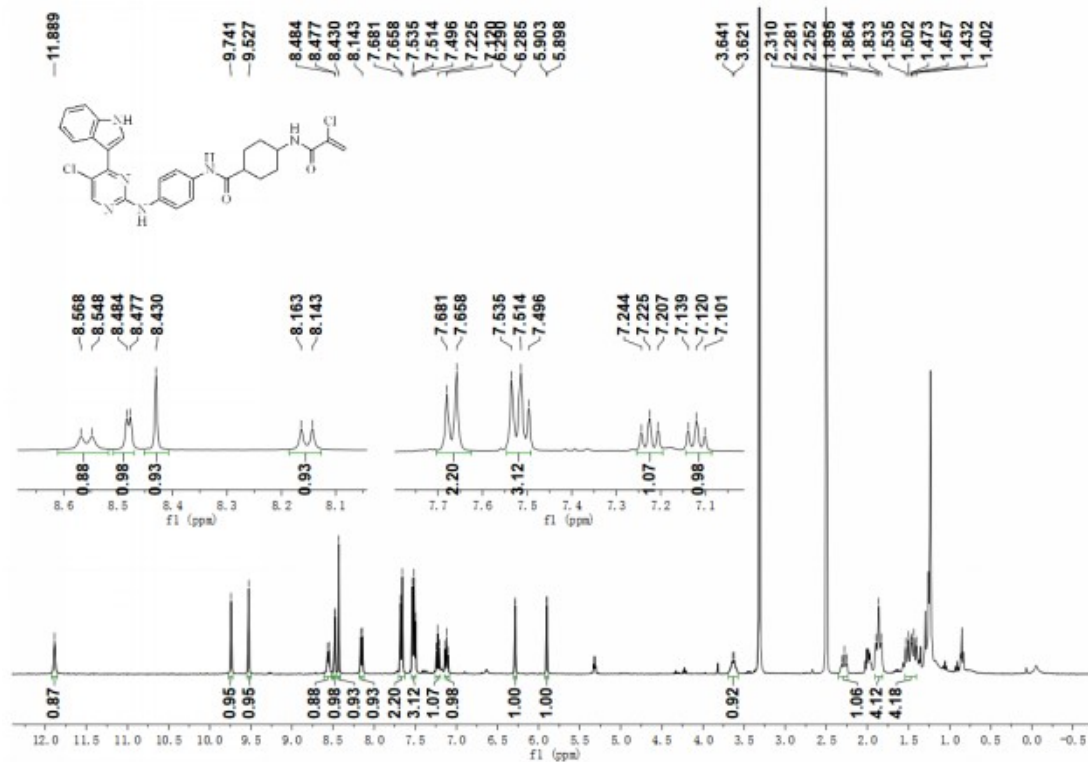
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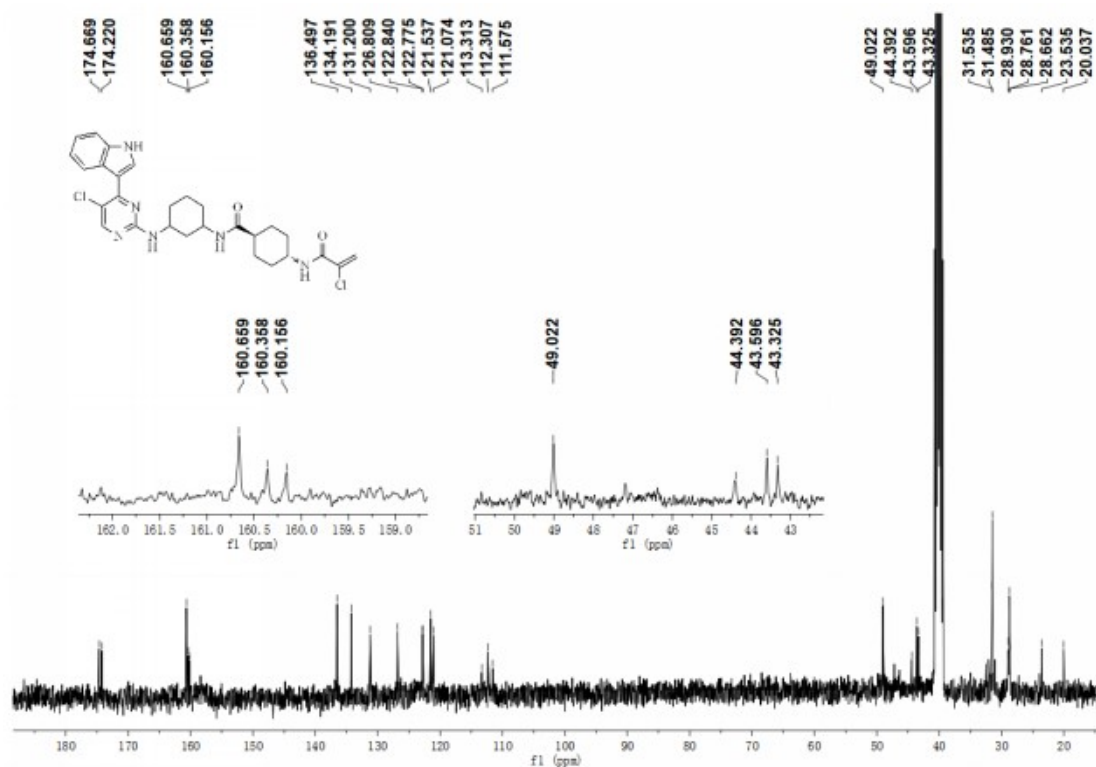
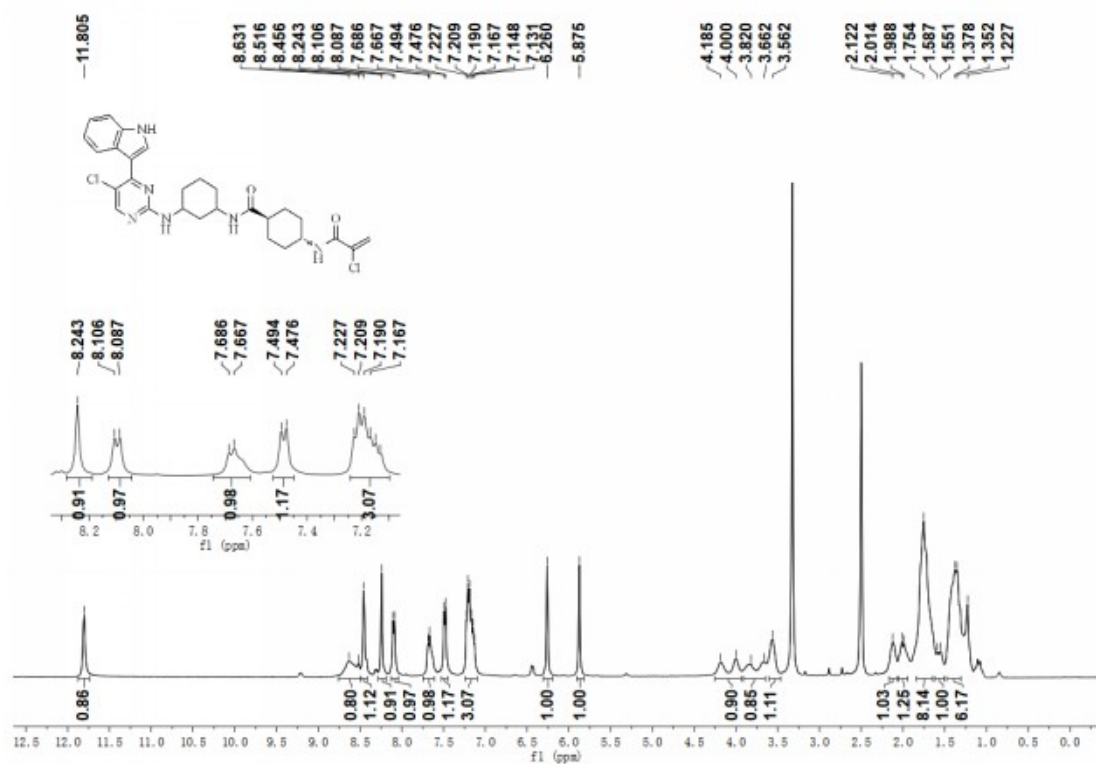
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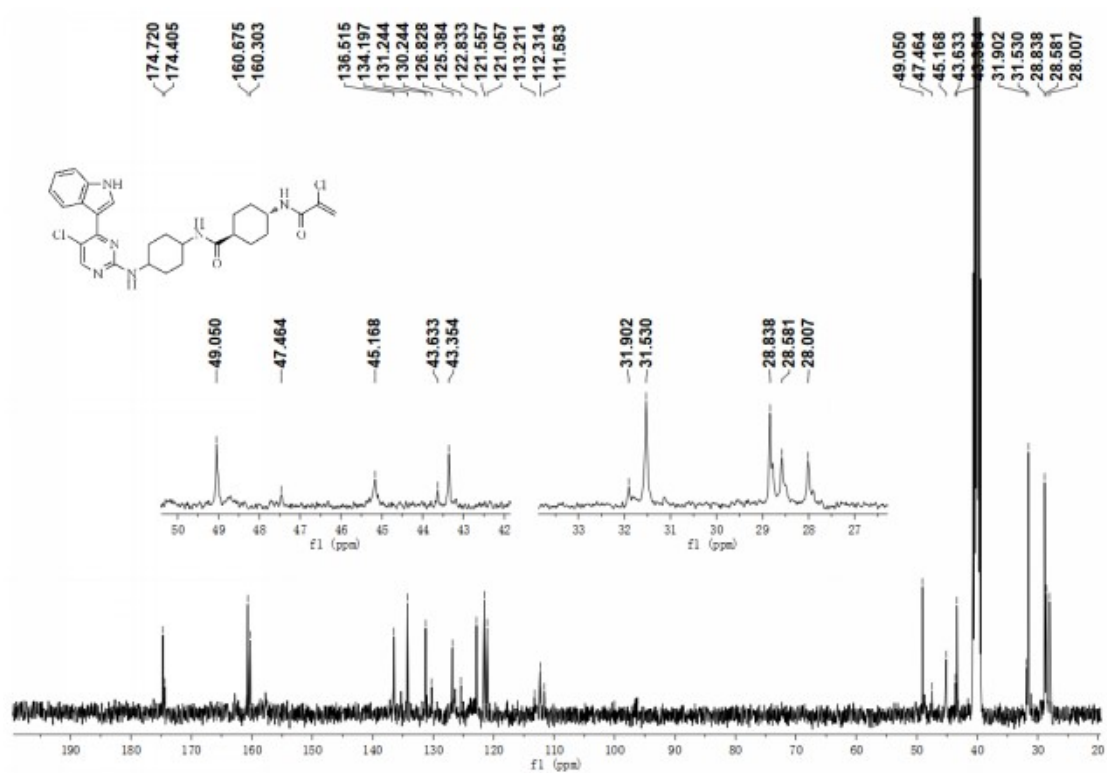
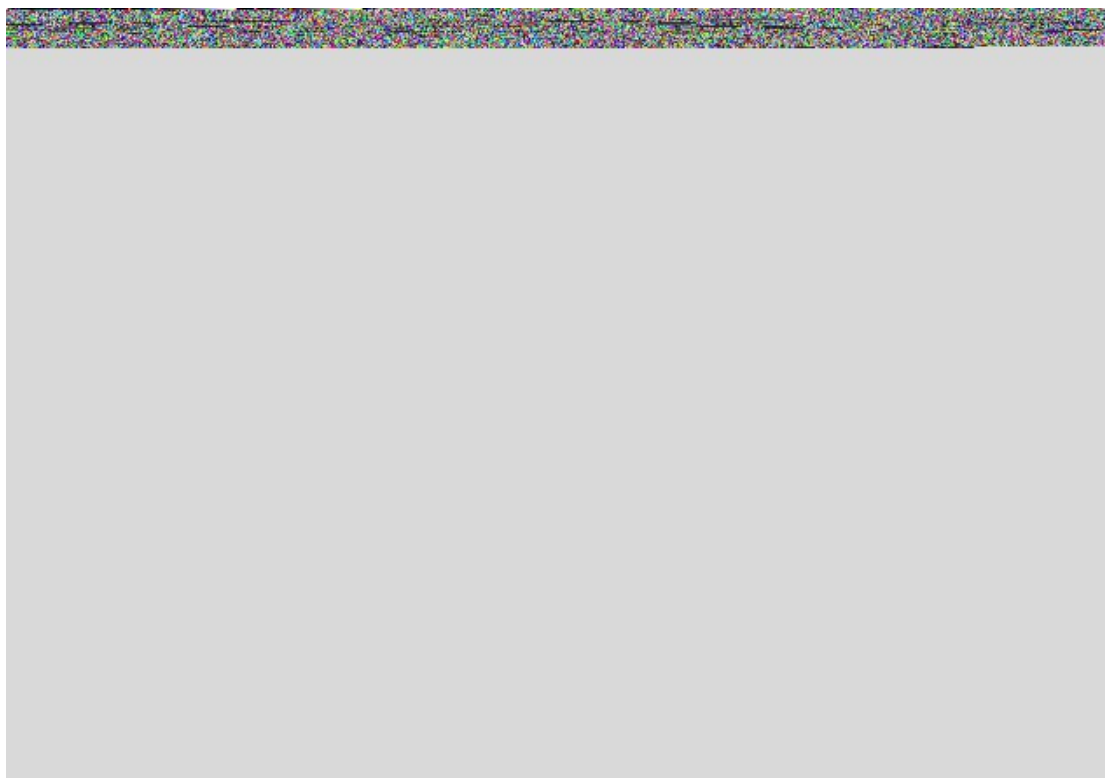
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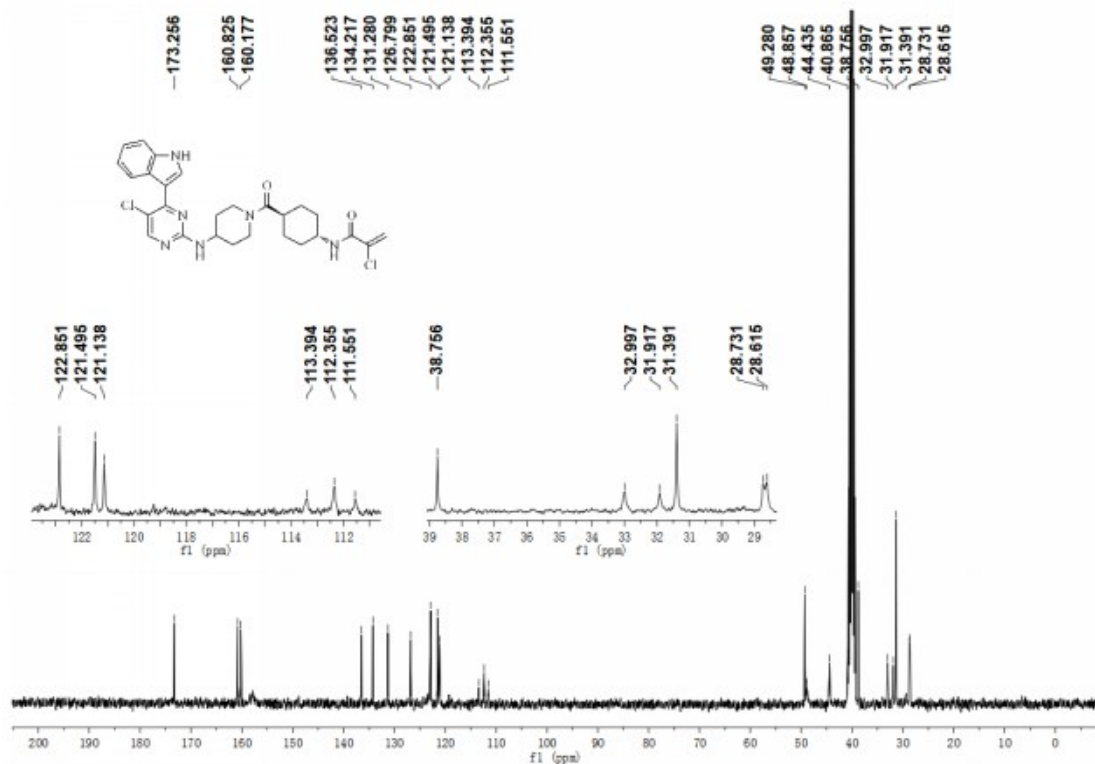
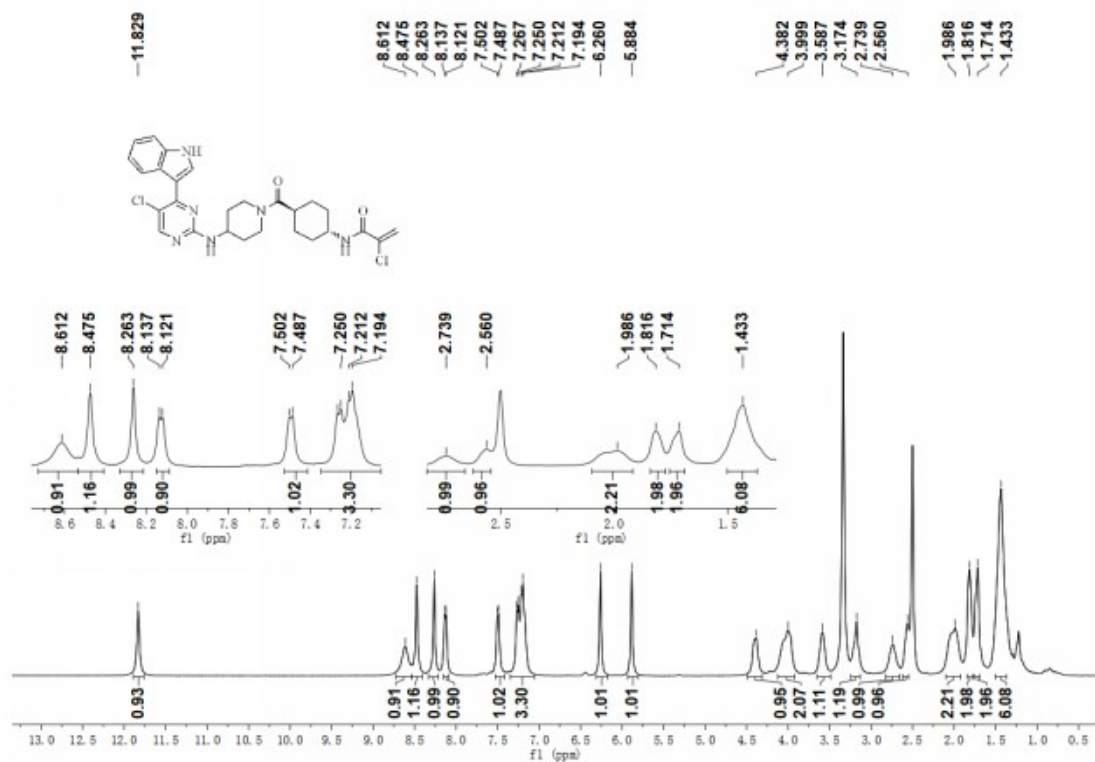
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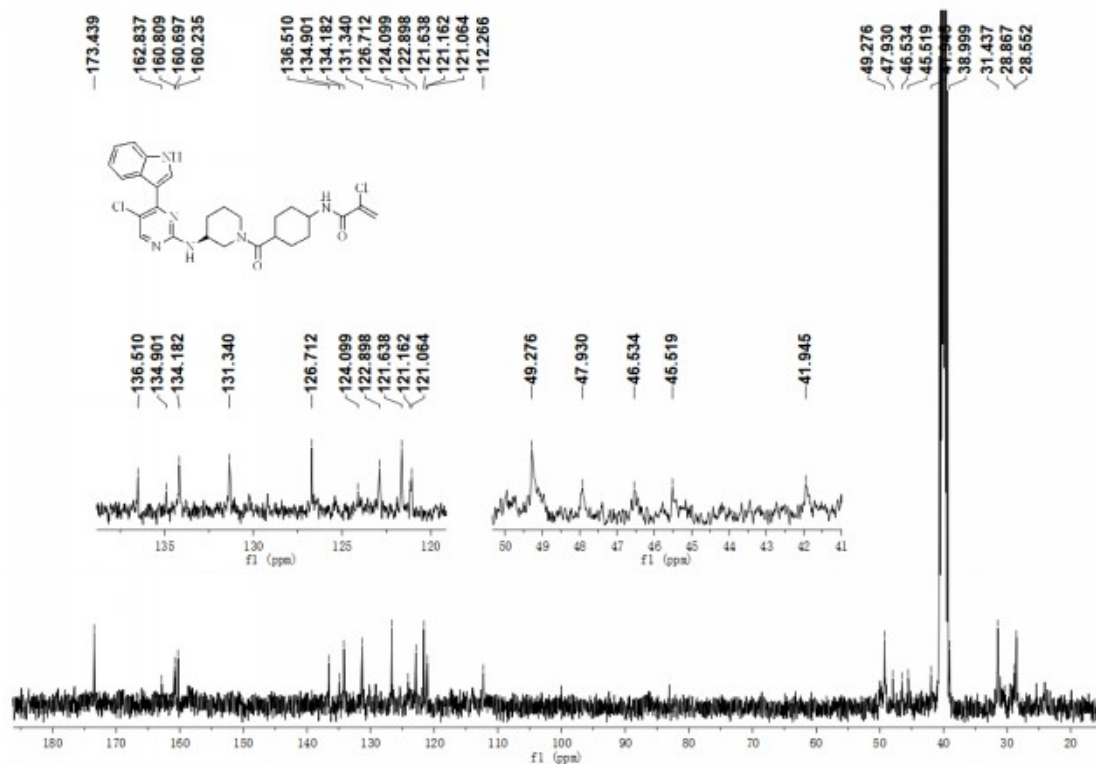
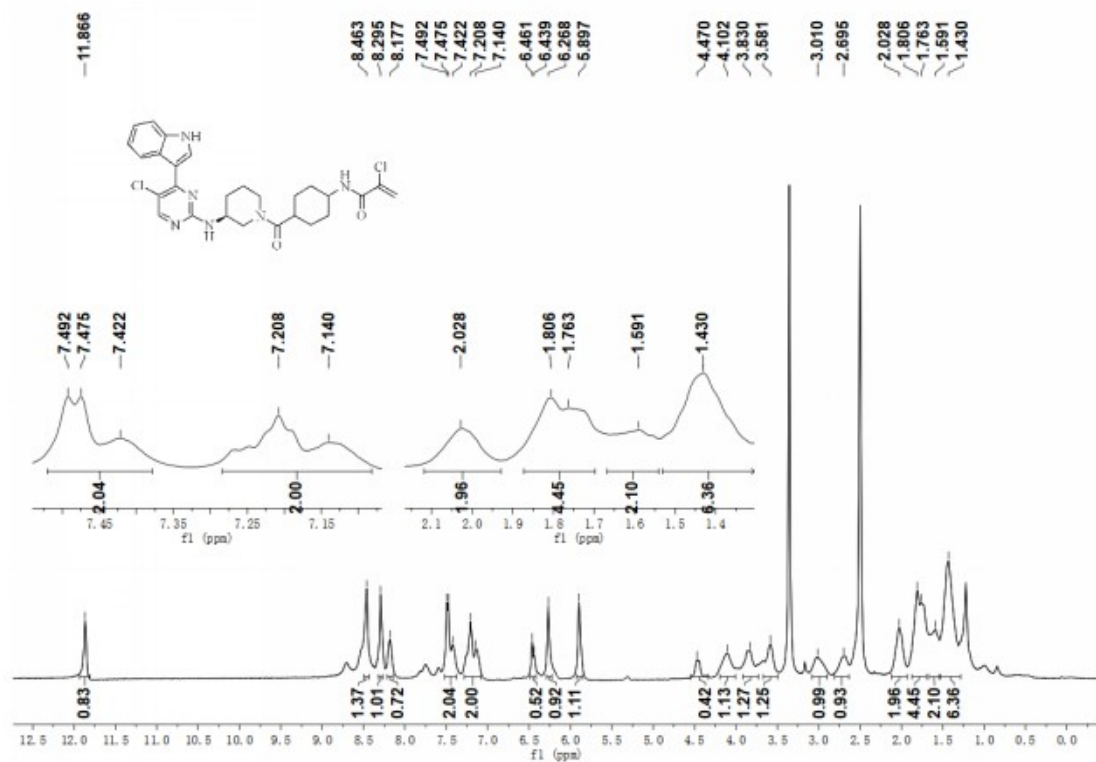
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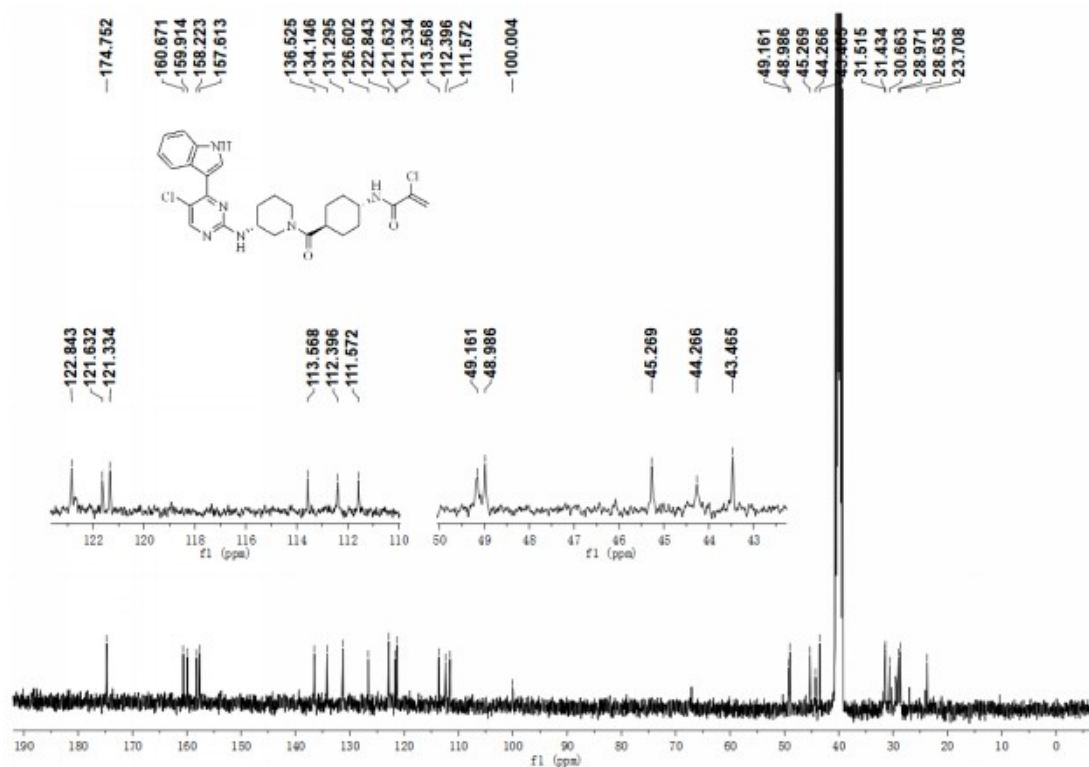
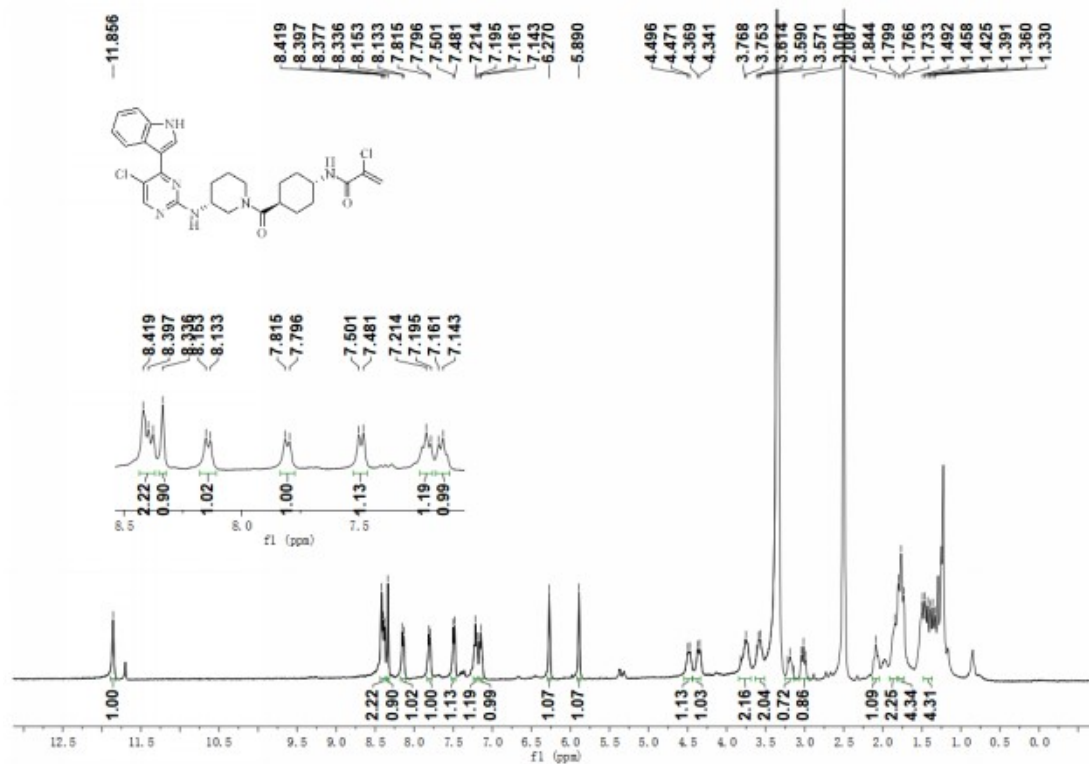
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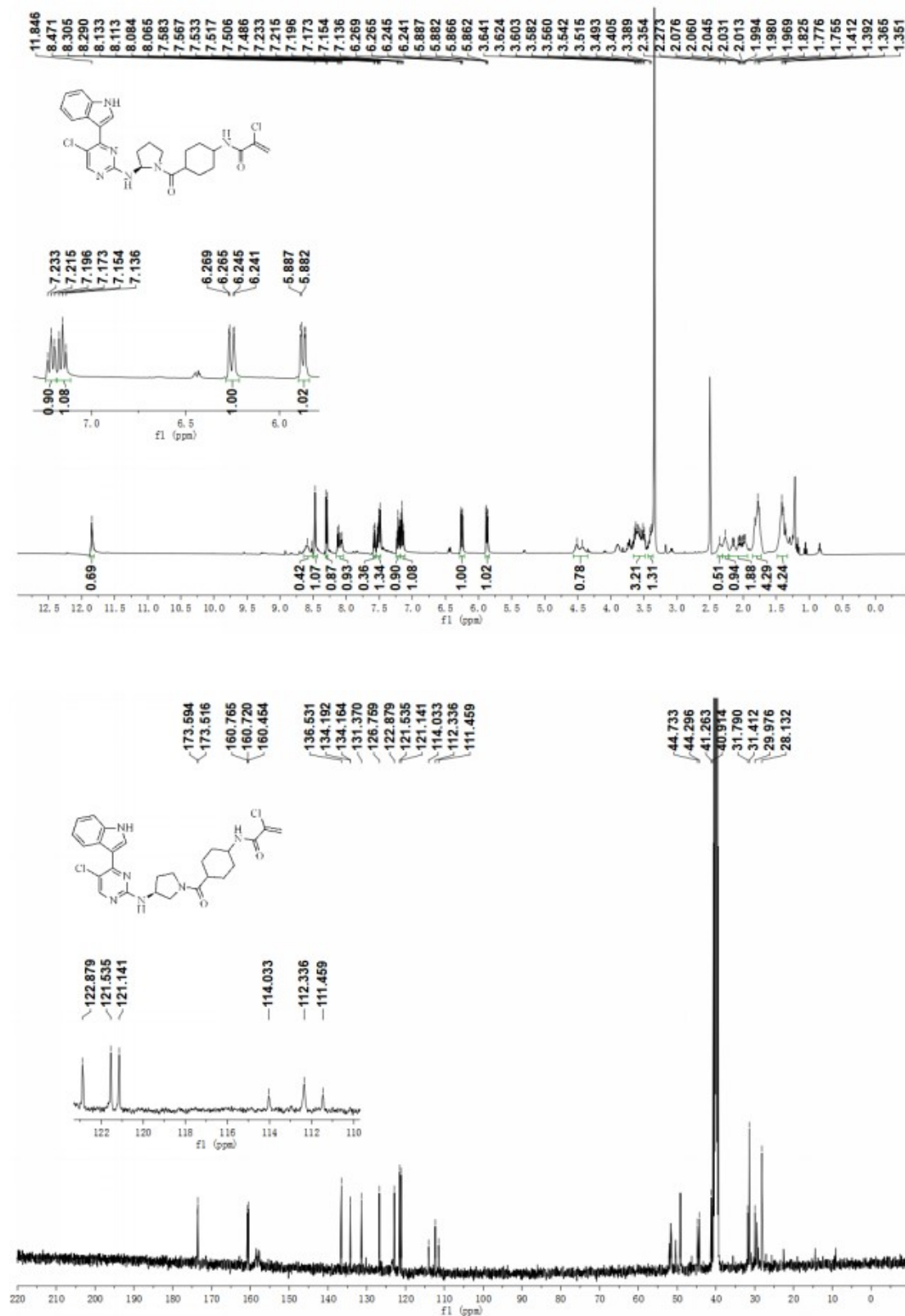
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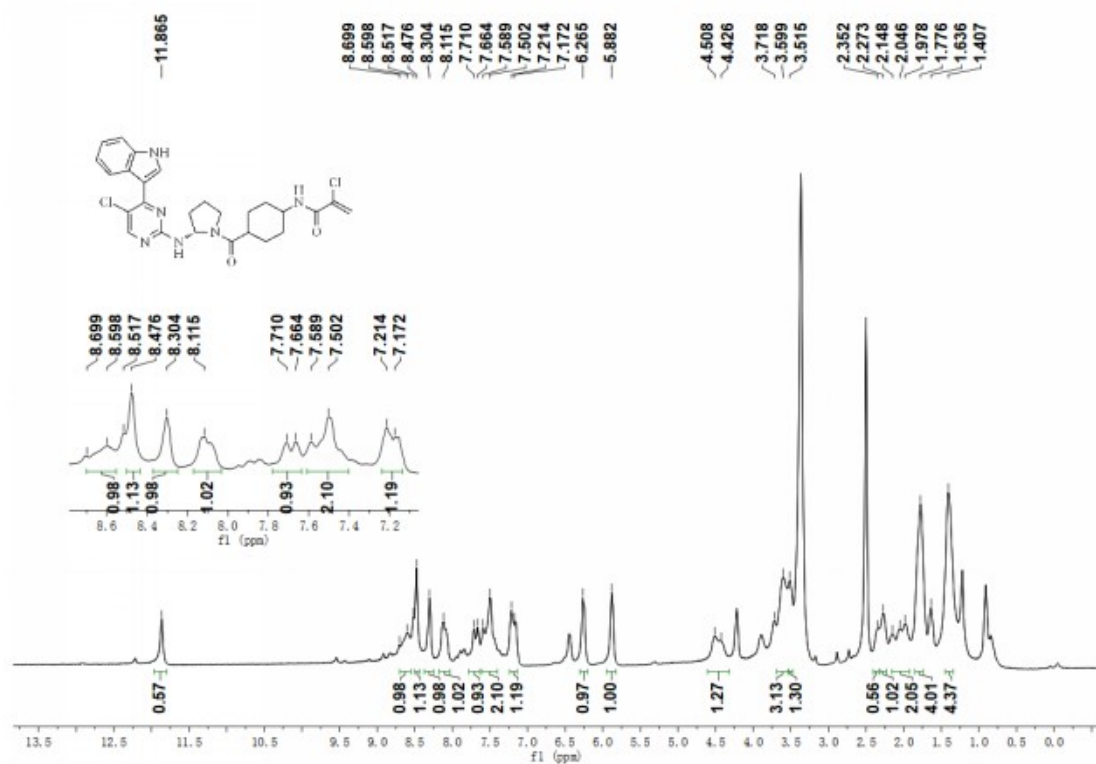
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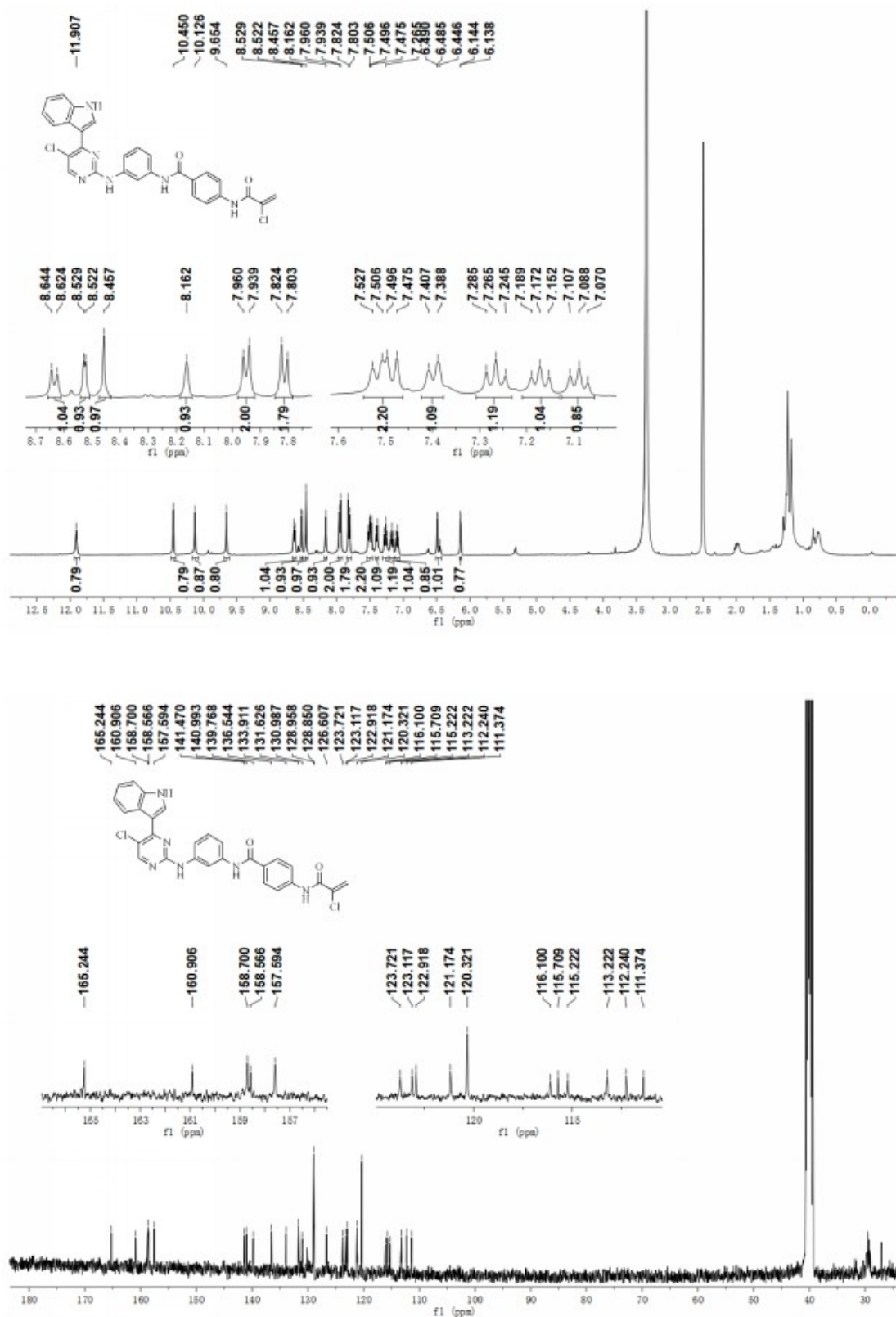
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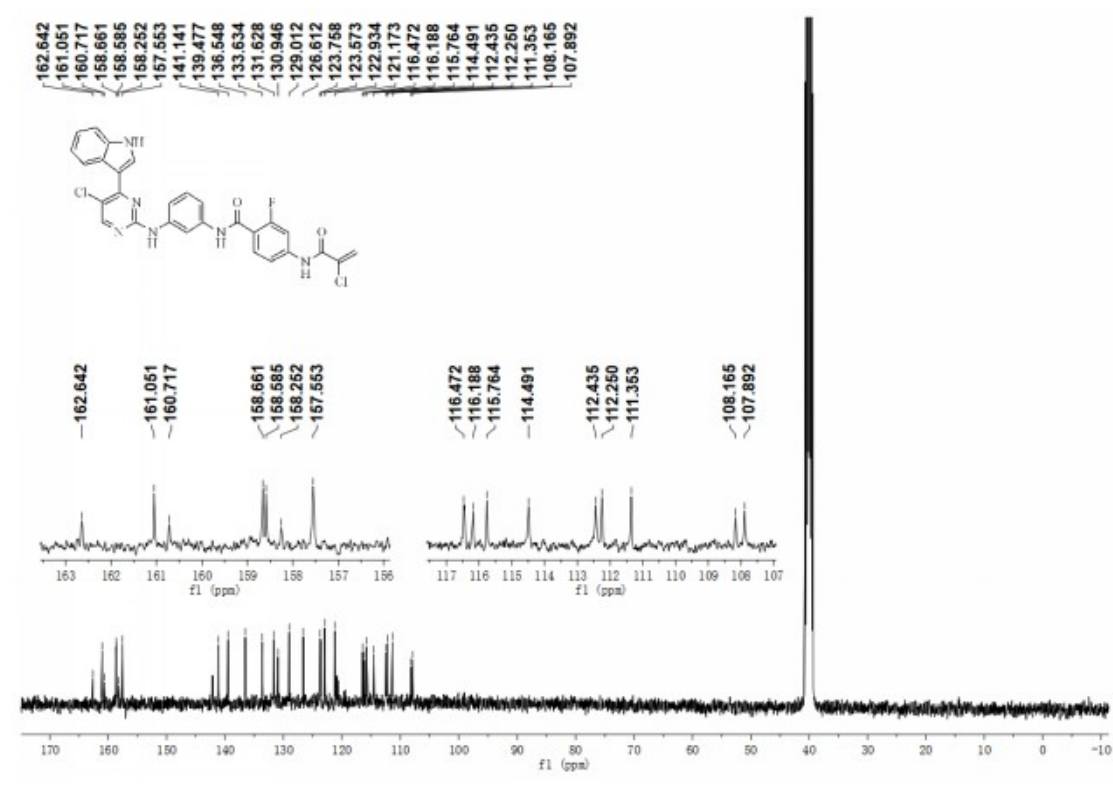
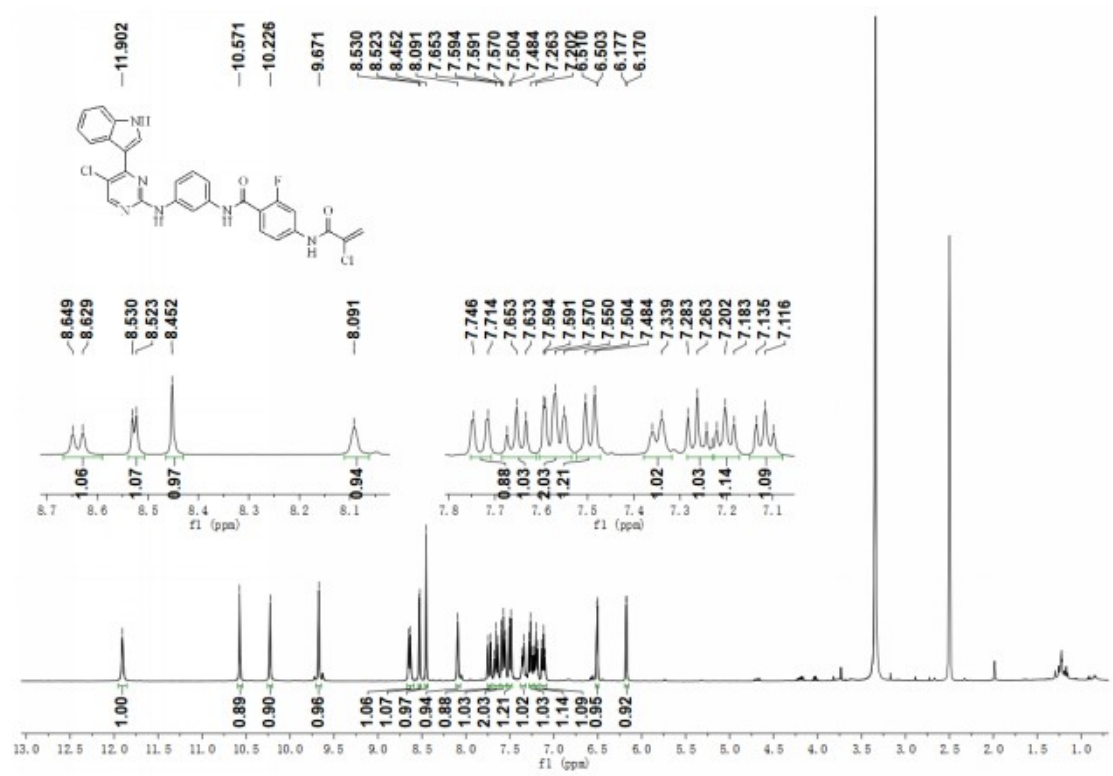
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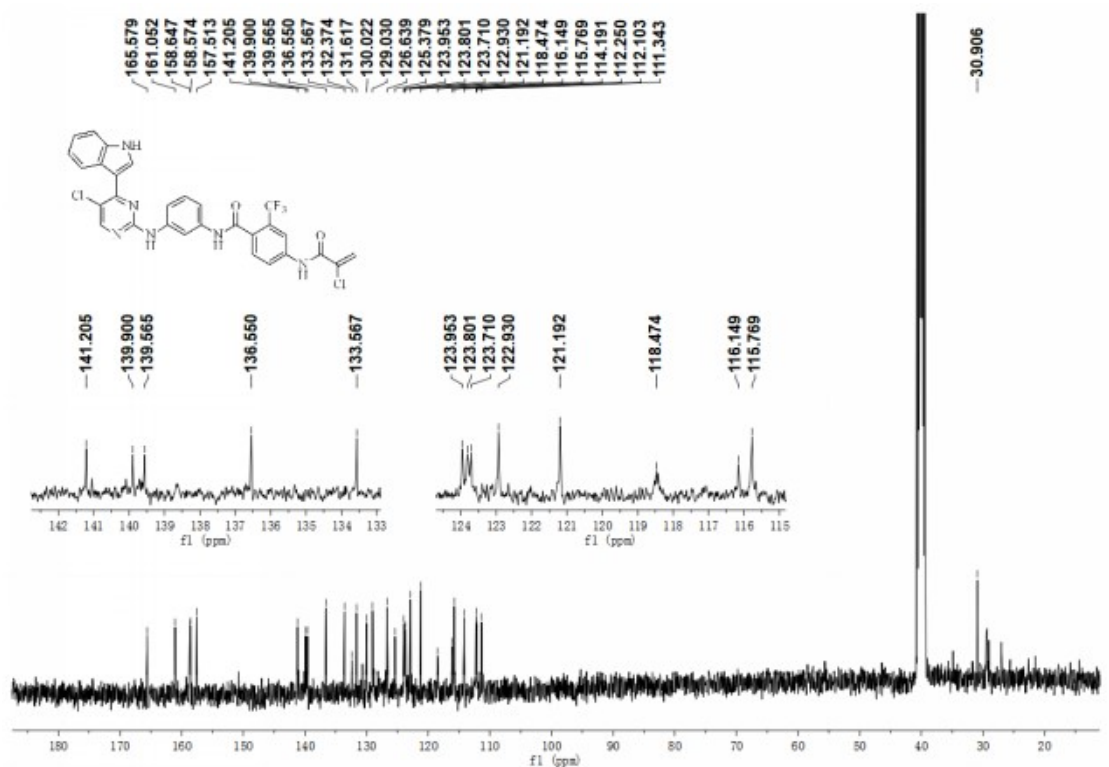
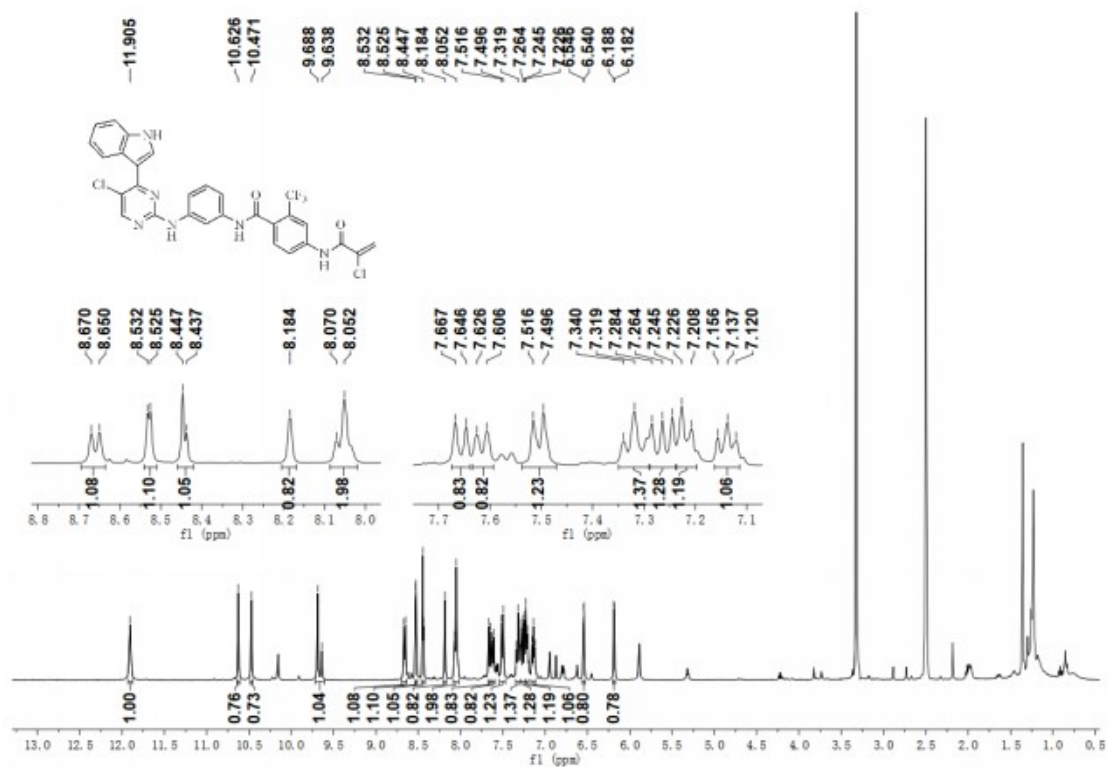
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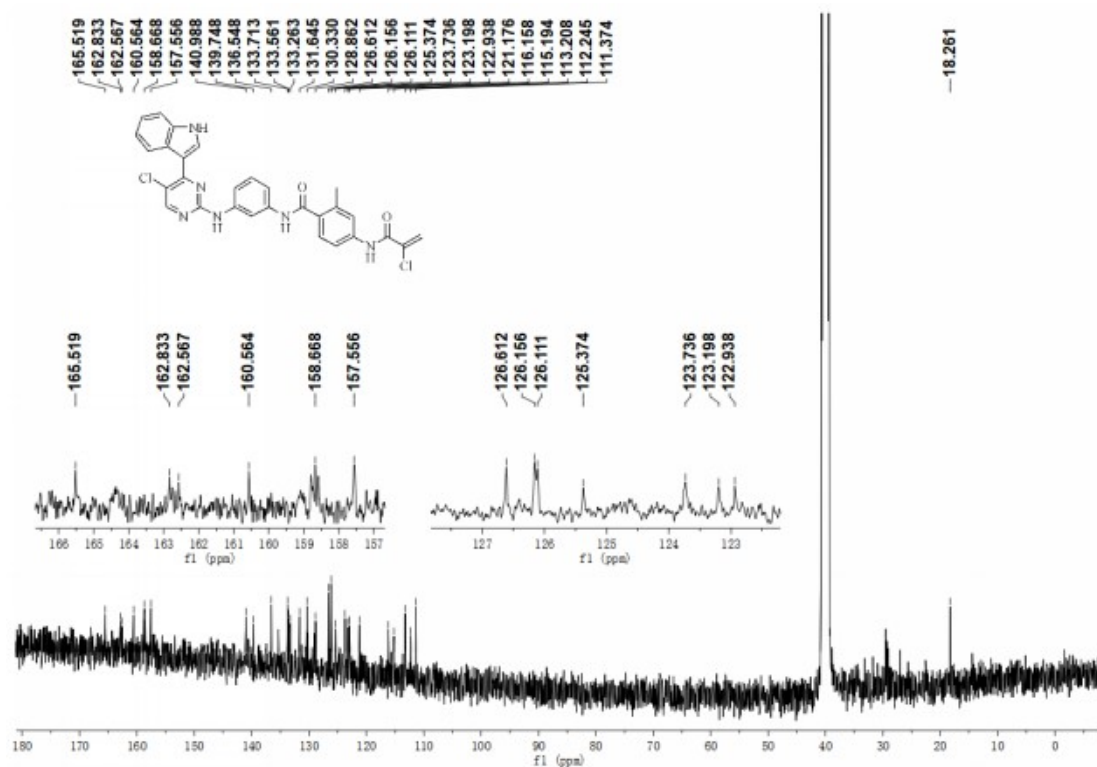
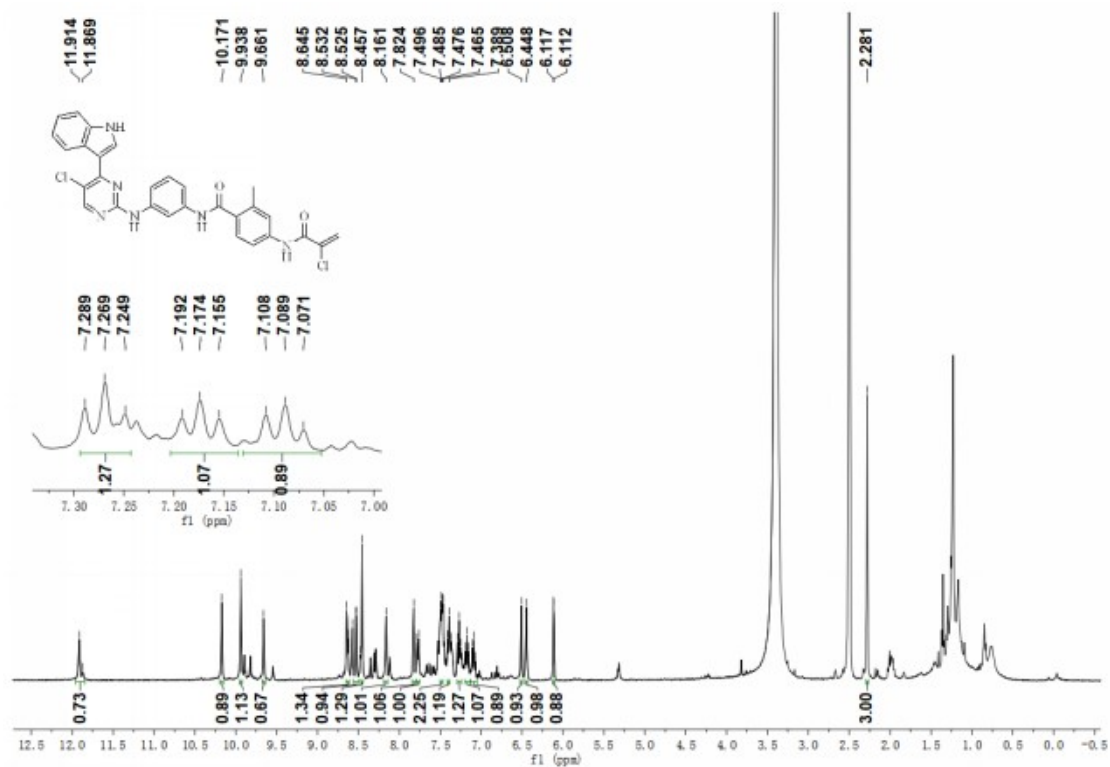
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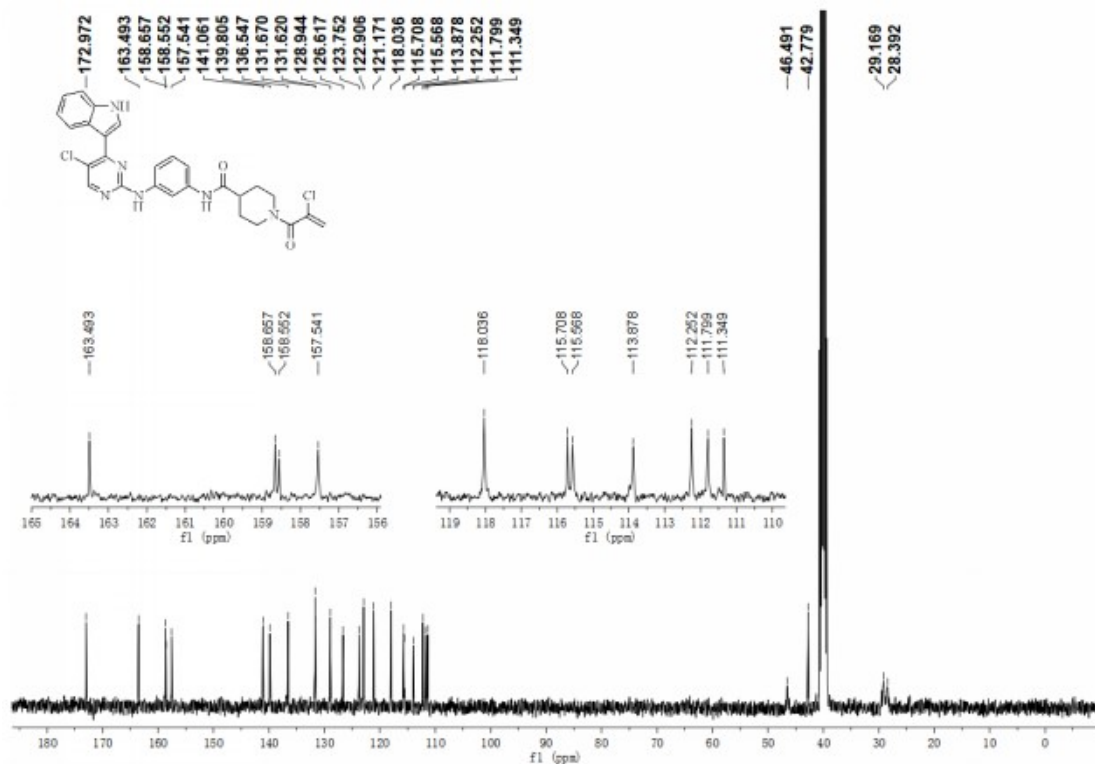
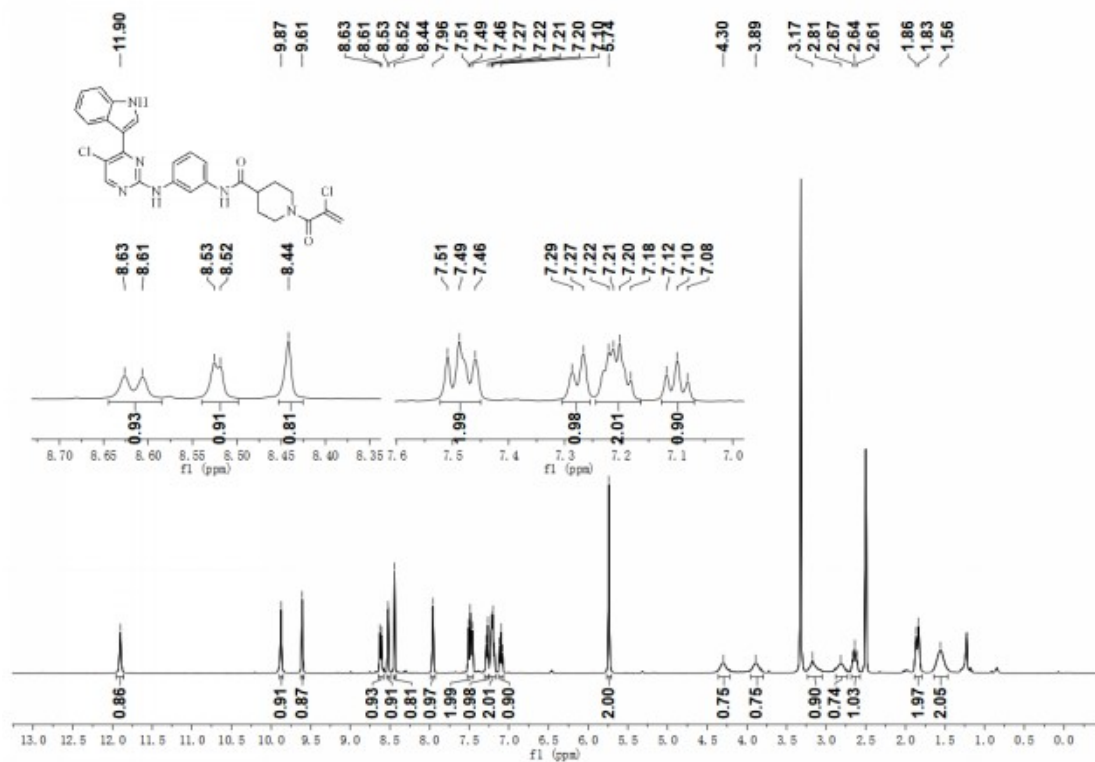
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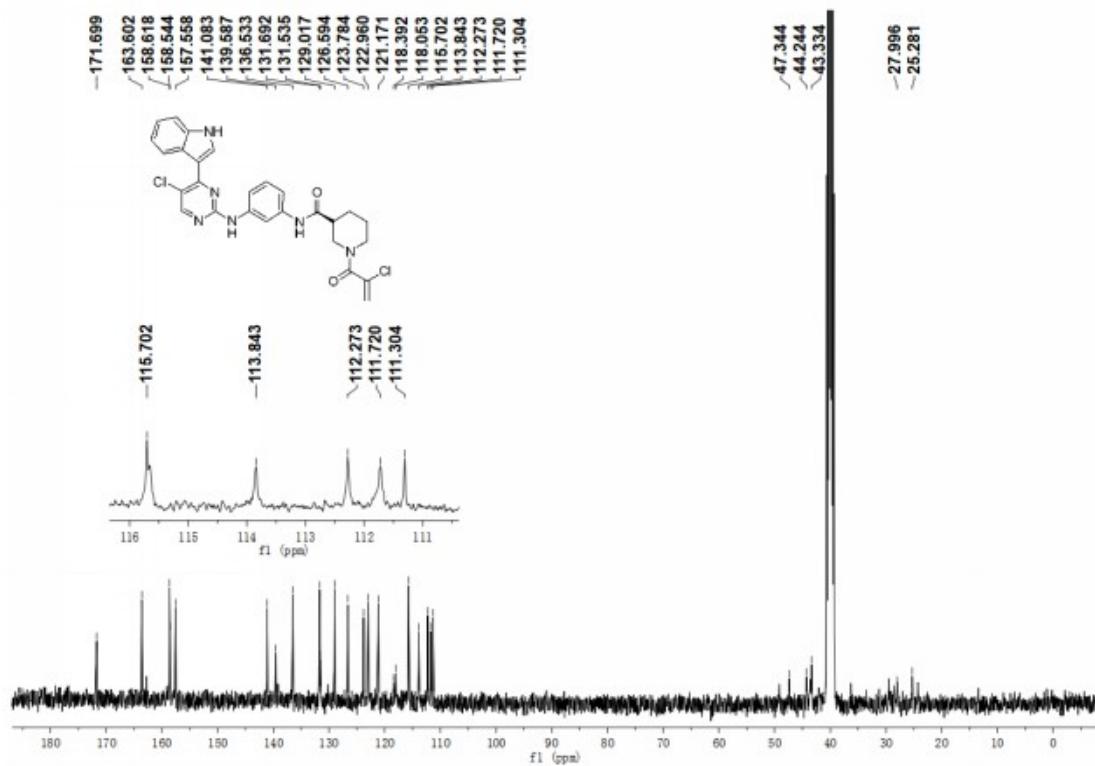
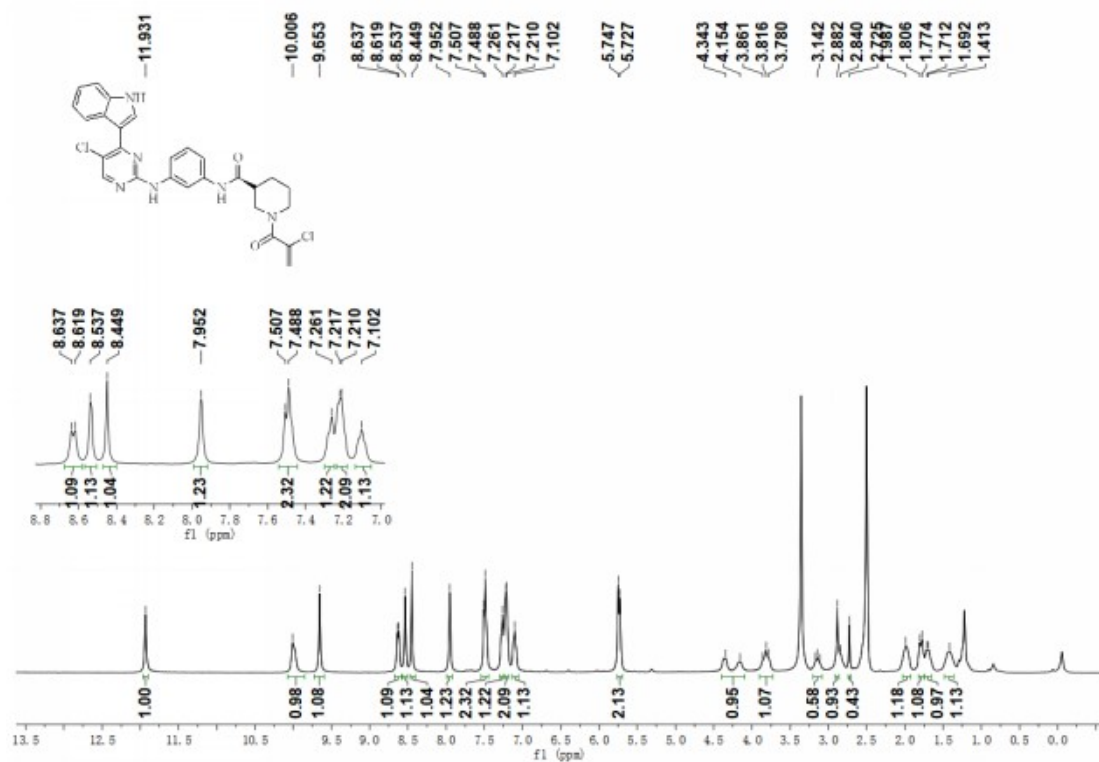
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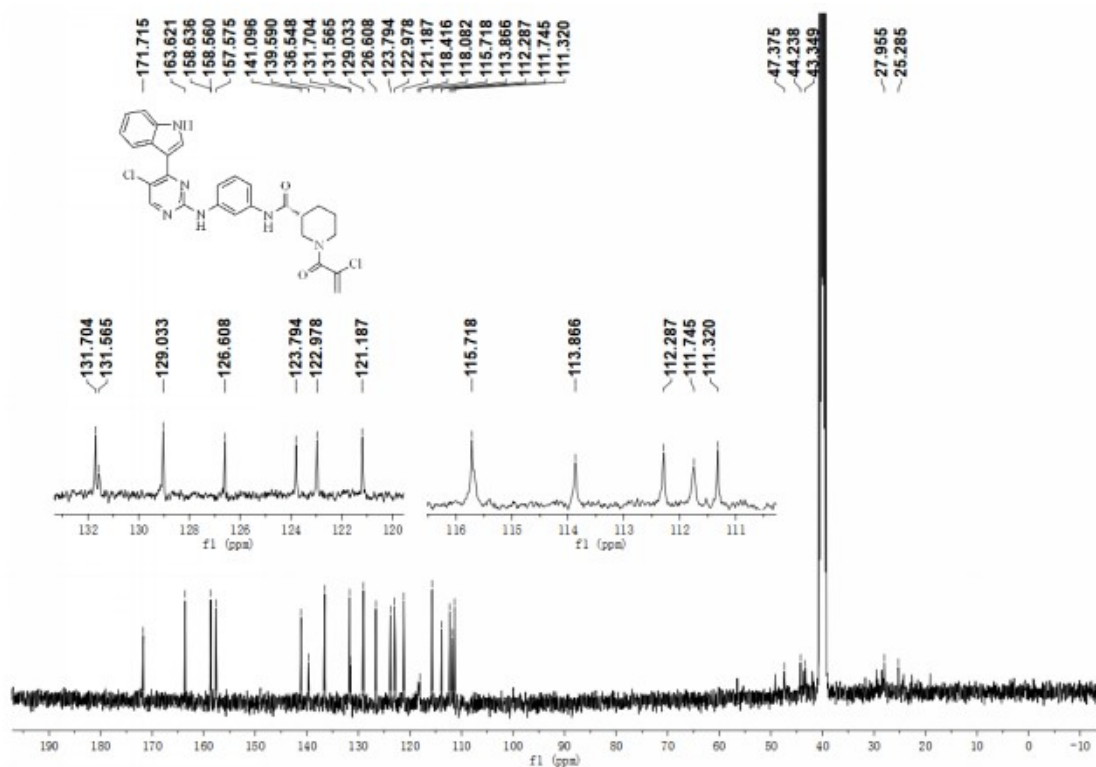
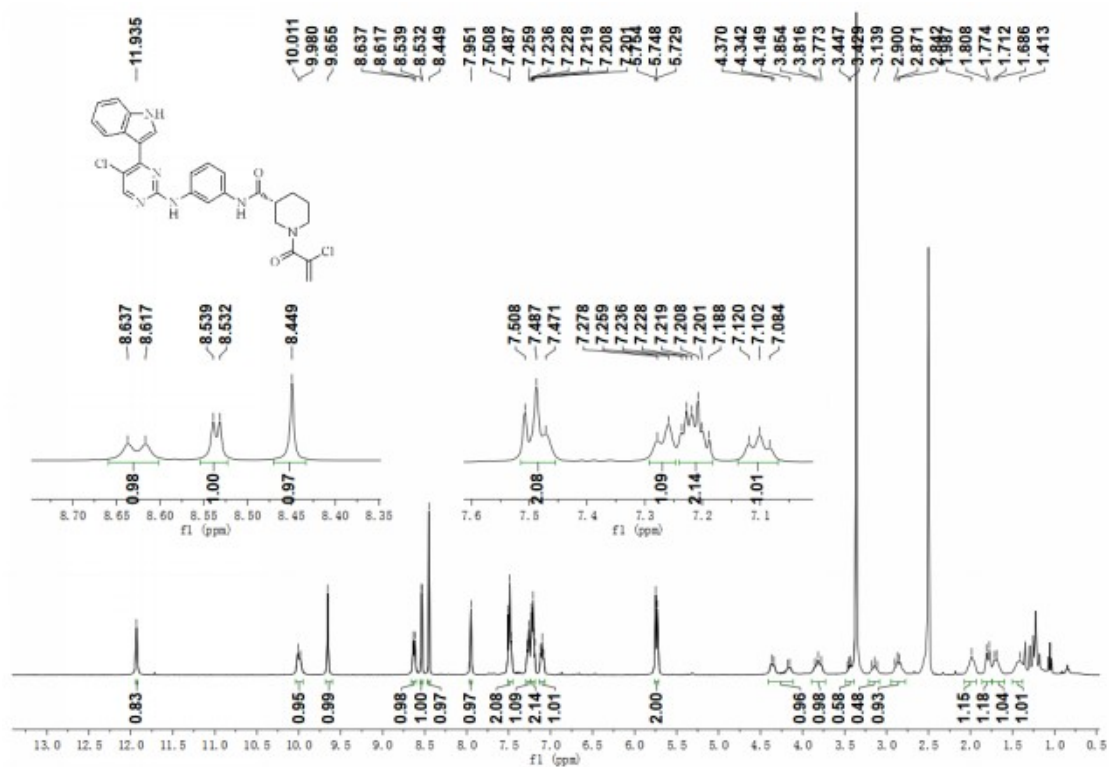
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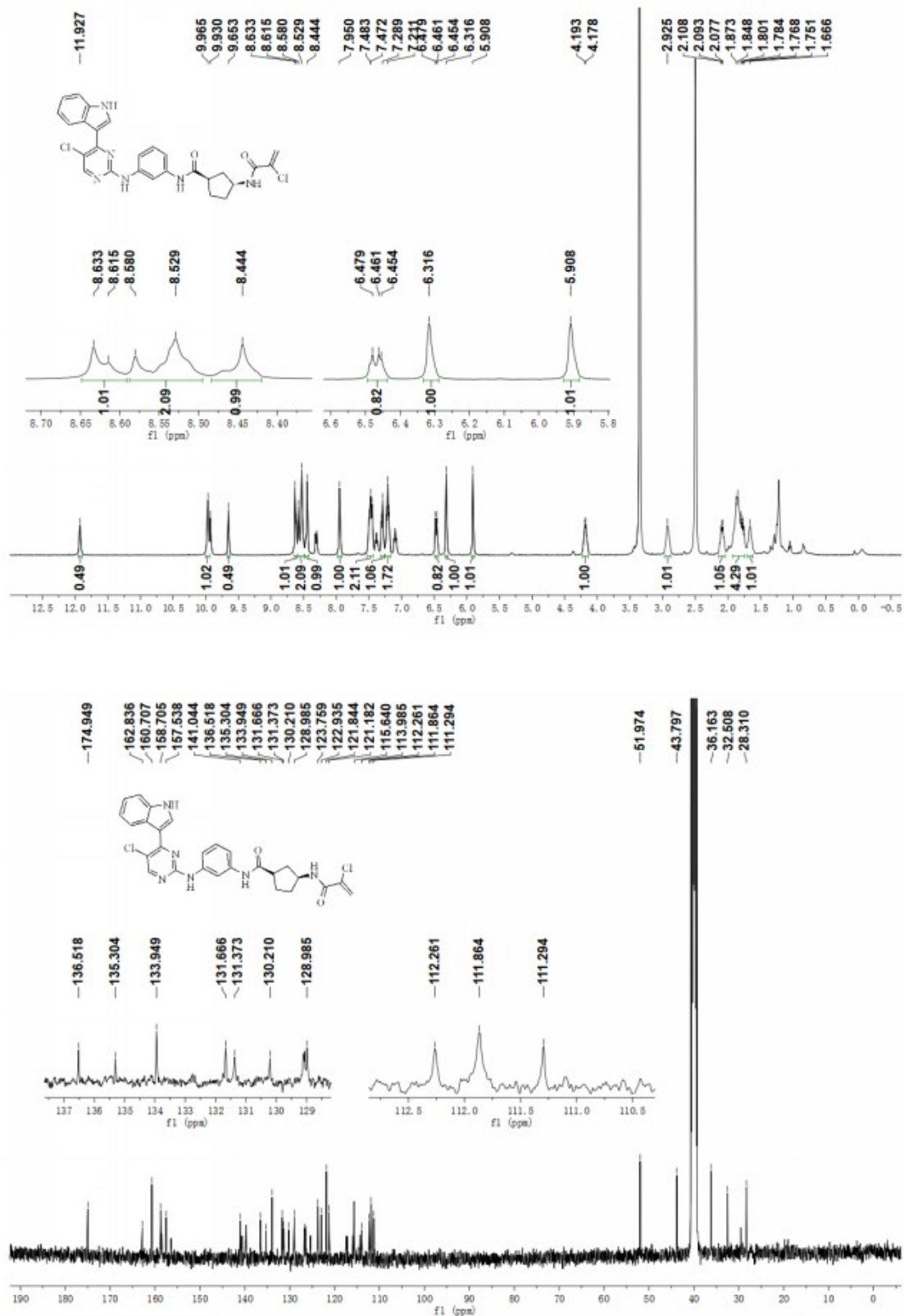
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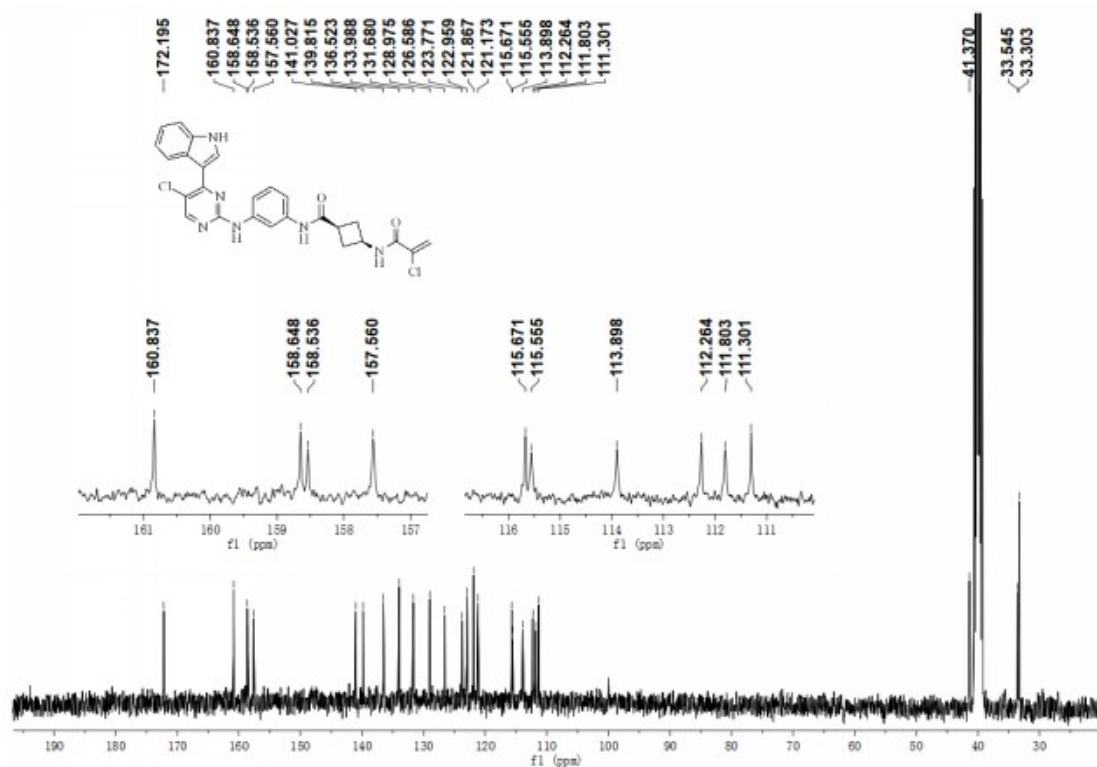
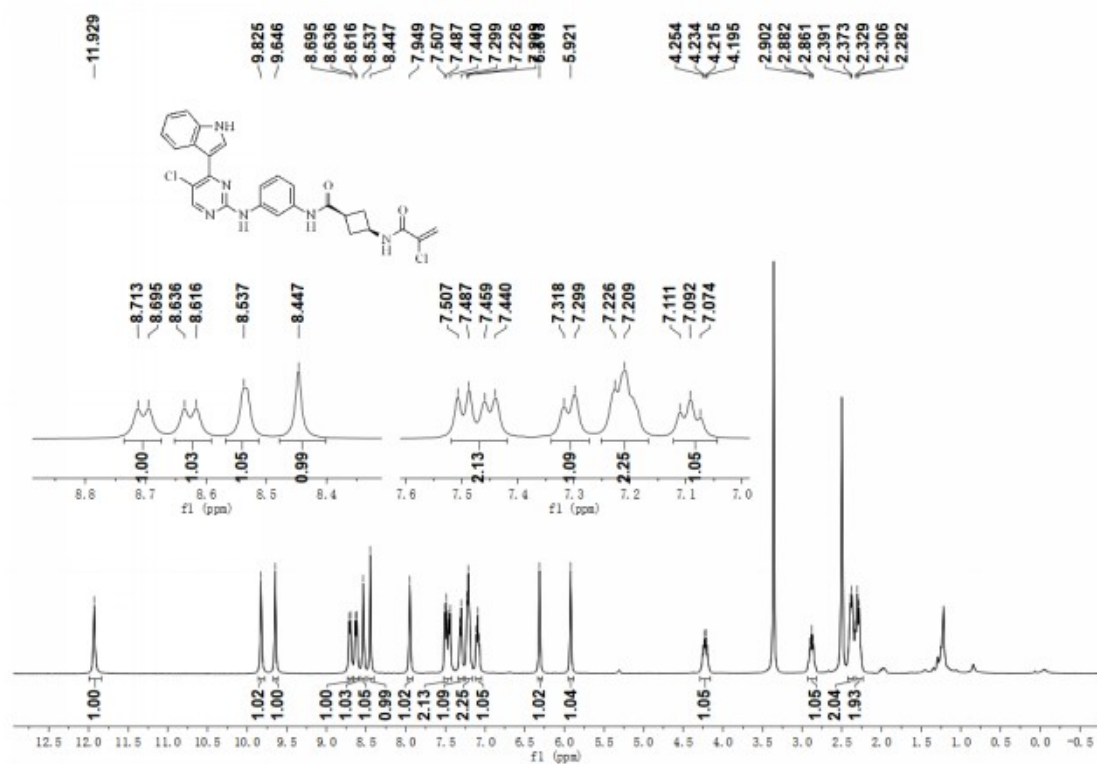
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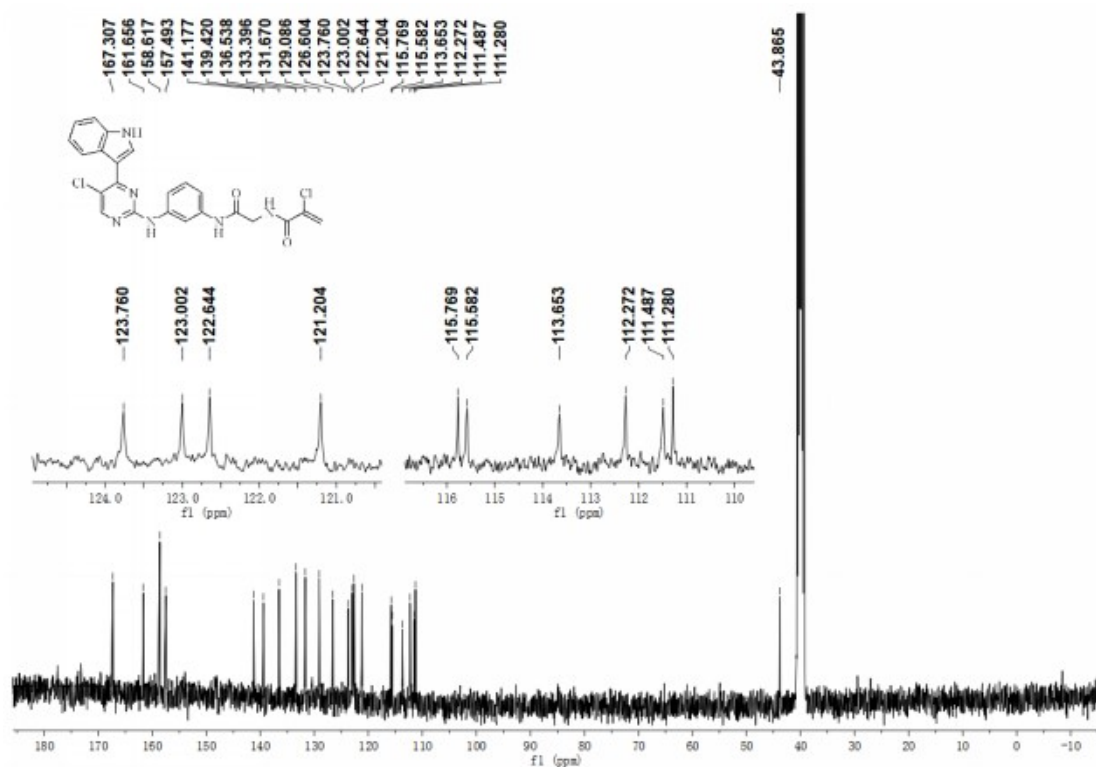
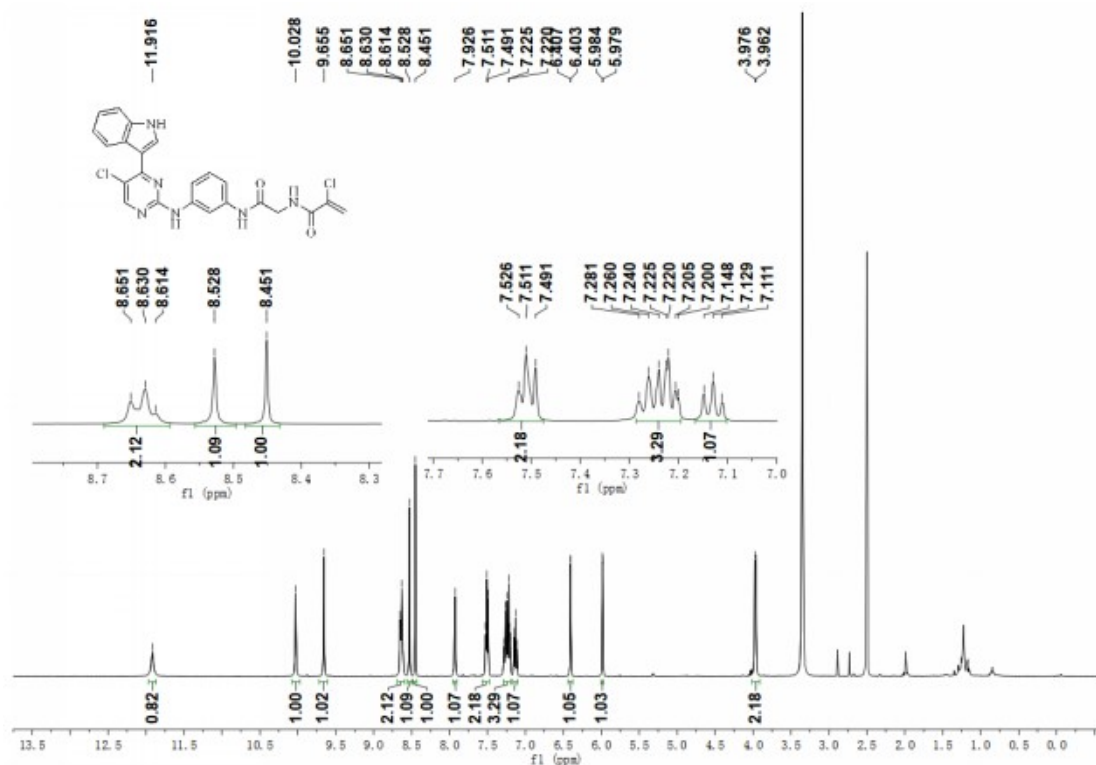
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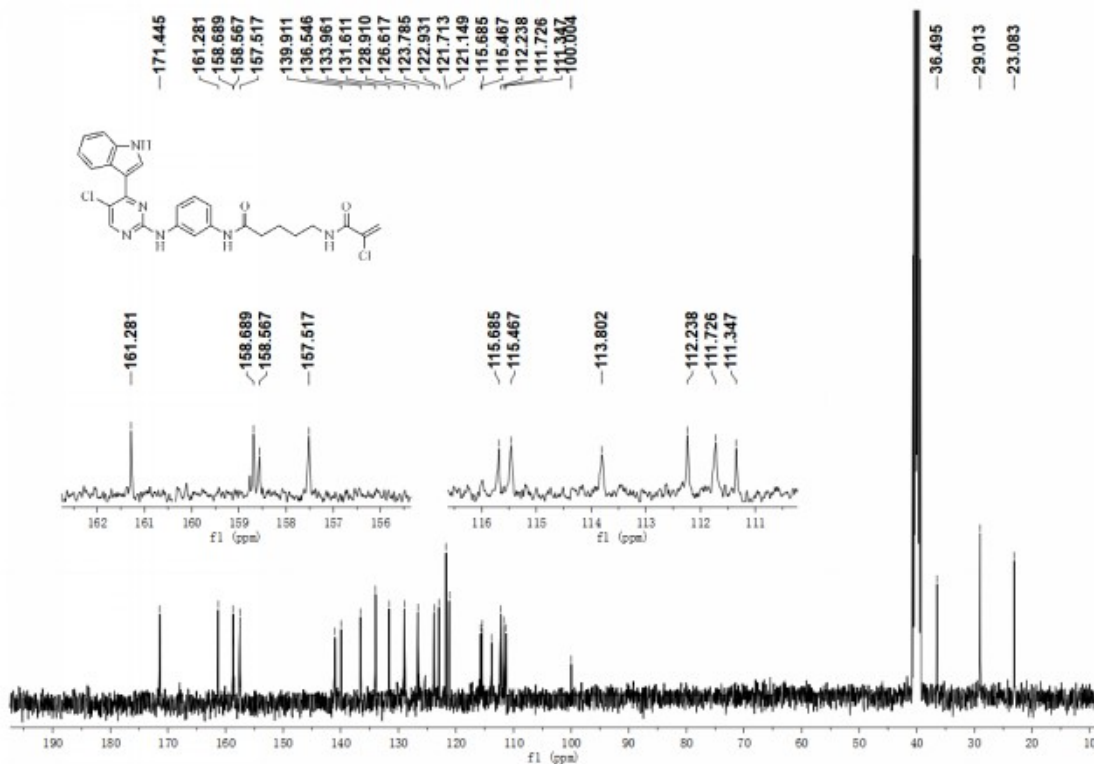
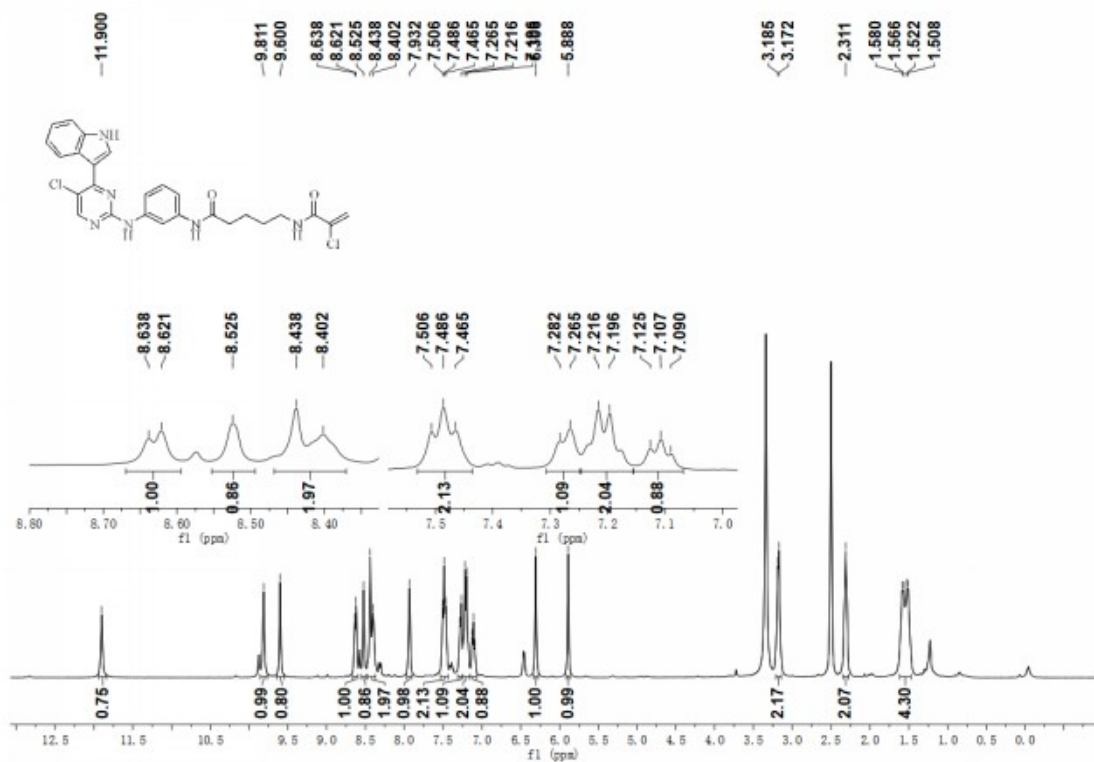
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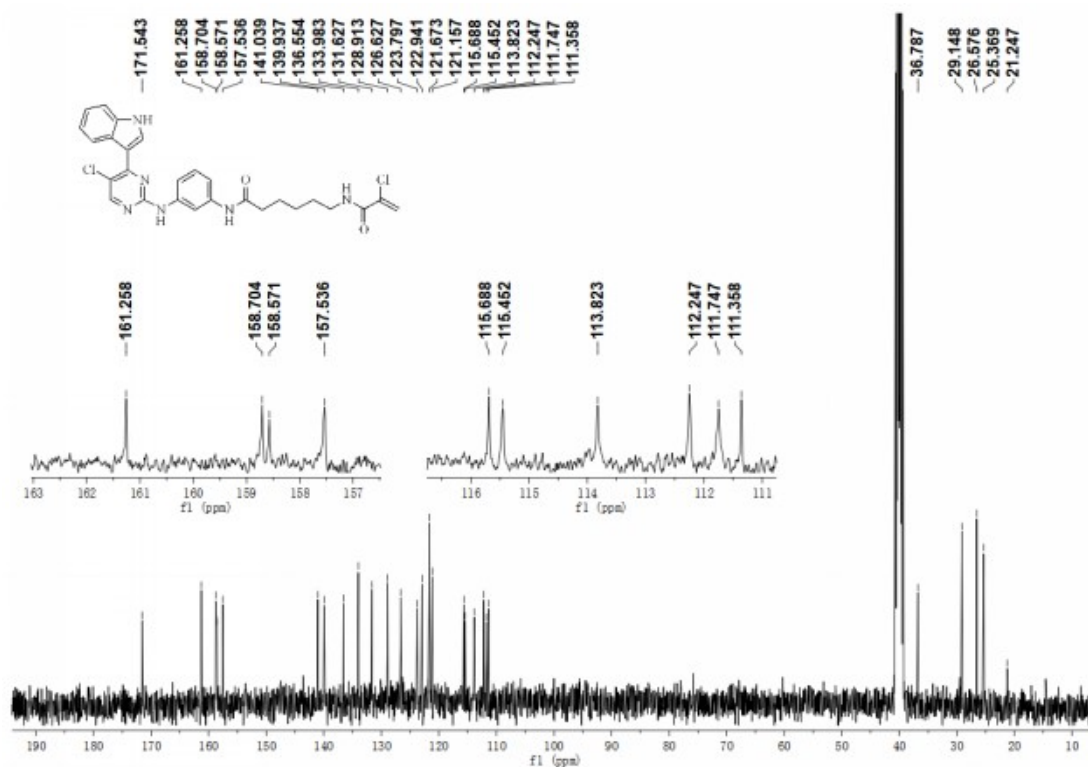
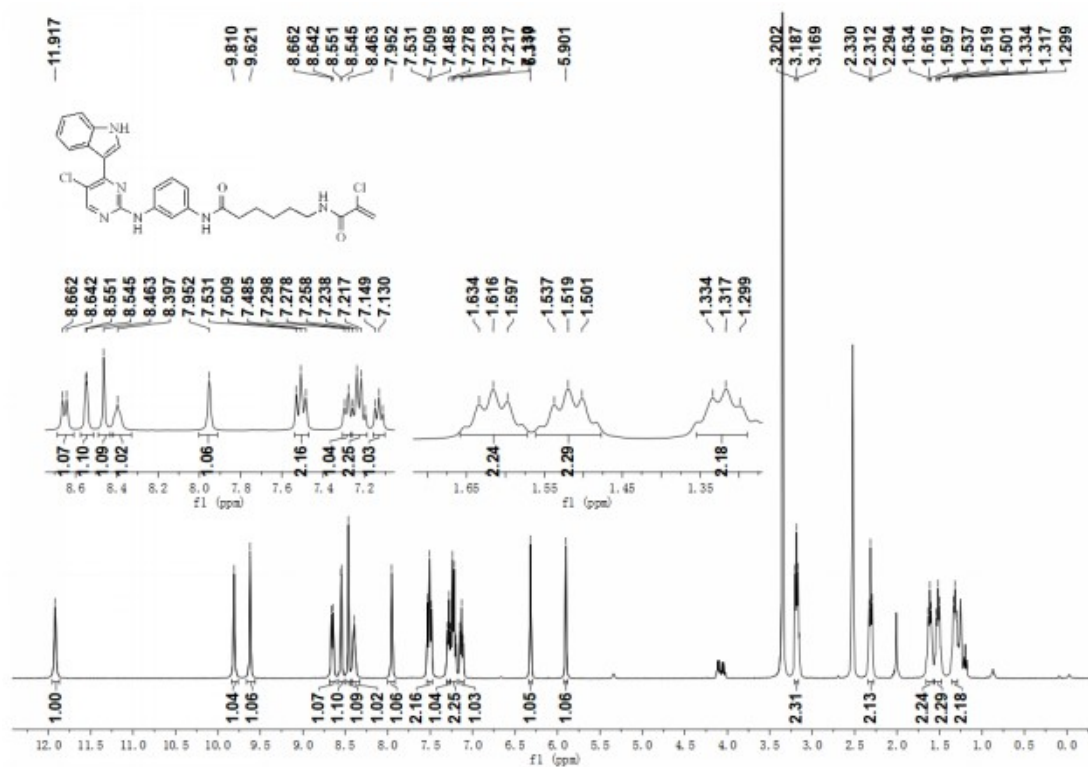
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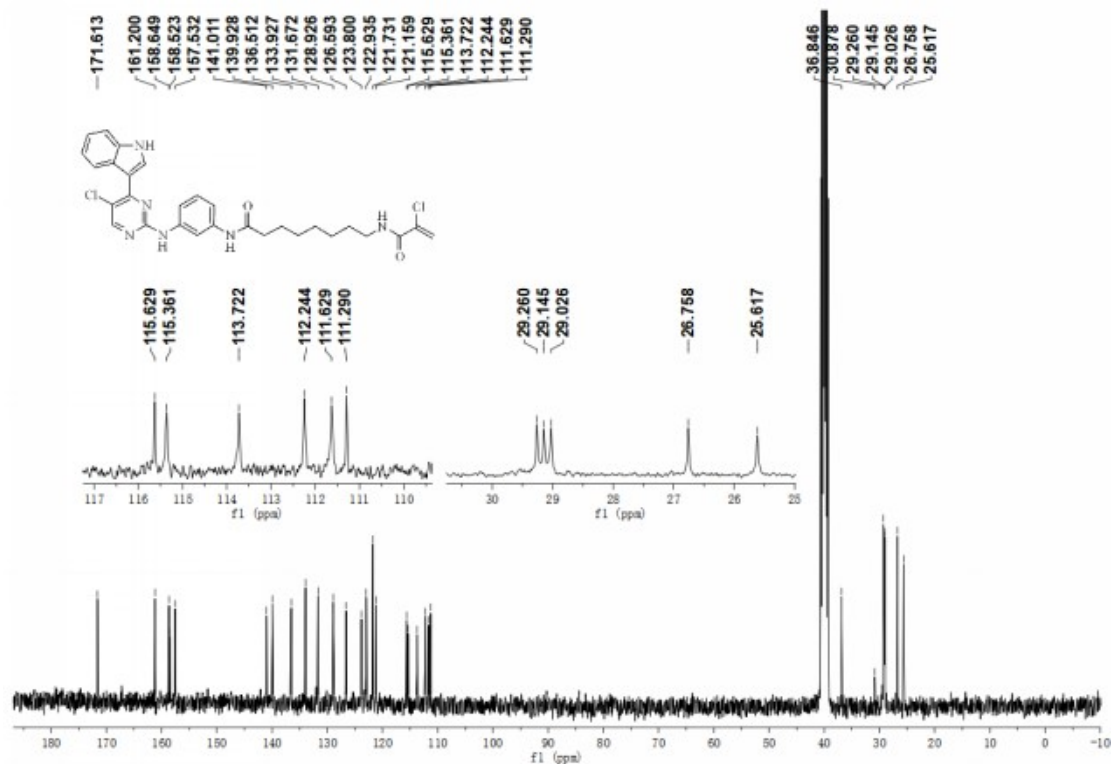
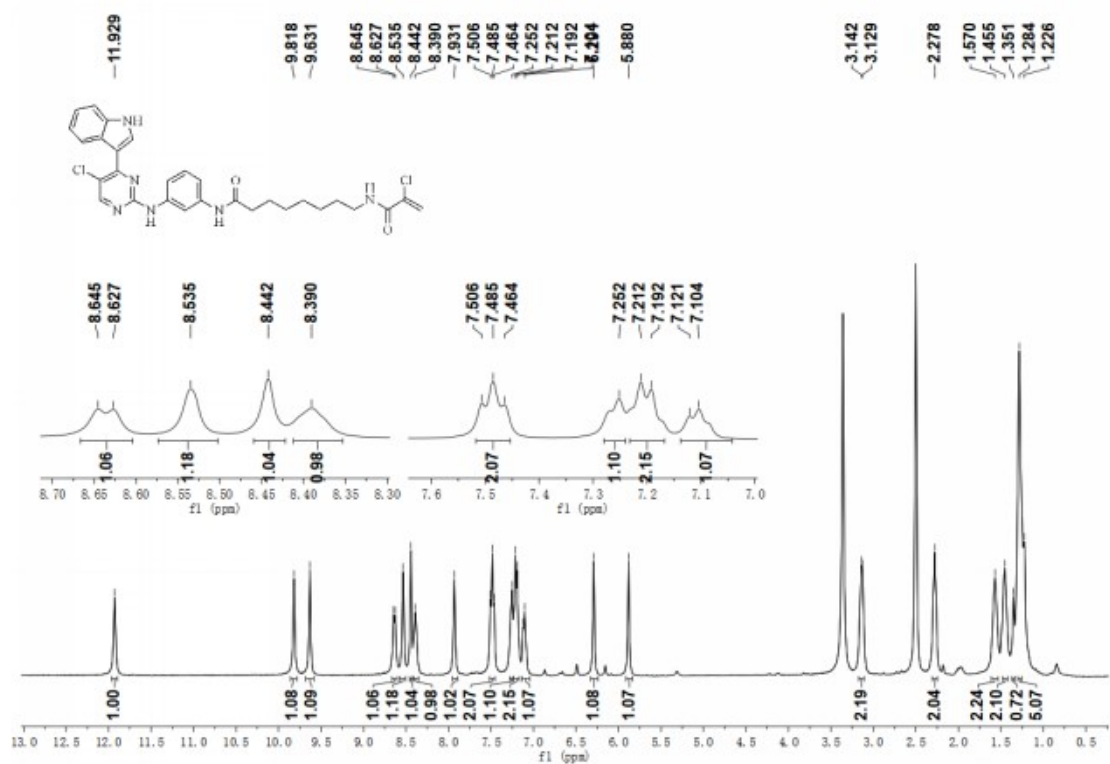
^1H NMR and ^{13}C NMR spectra of **B21** in $\text{DMSO-}d_6$



^1H NMR and ^{13}C NMR spectra of **B22** in $\text{DMSO-}d_6$



^1H NMR and ^{13}C NMR spectra of **B23** in $\text{DMSO-}d_6$



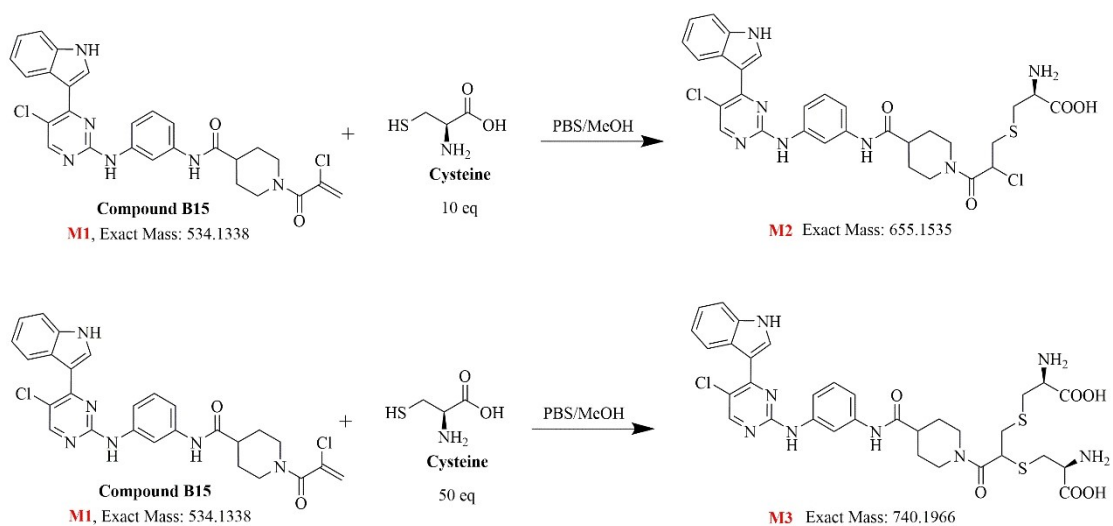


Figure S1. Covalent bond formation of B15 and Cysteine residue.

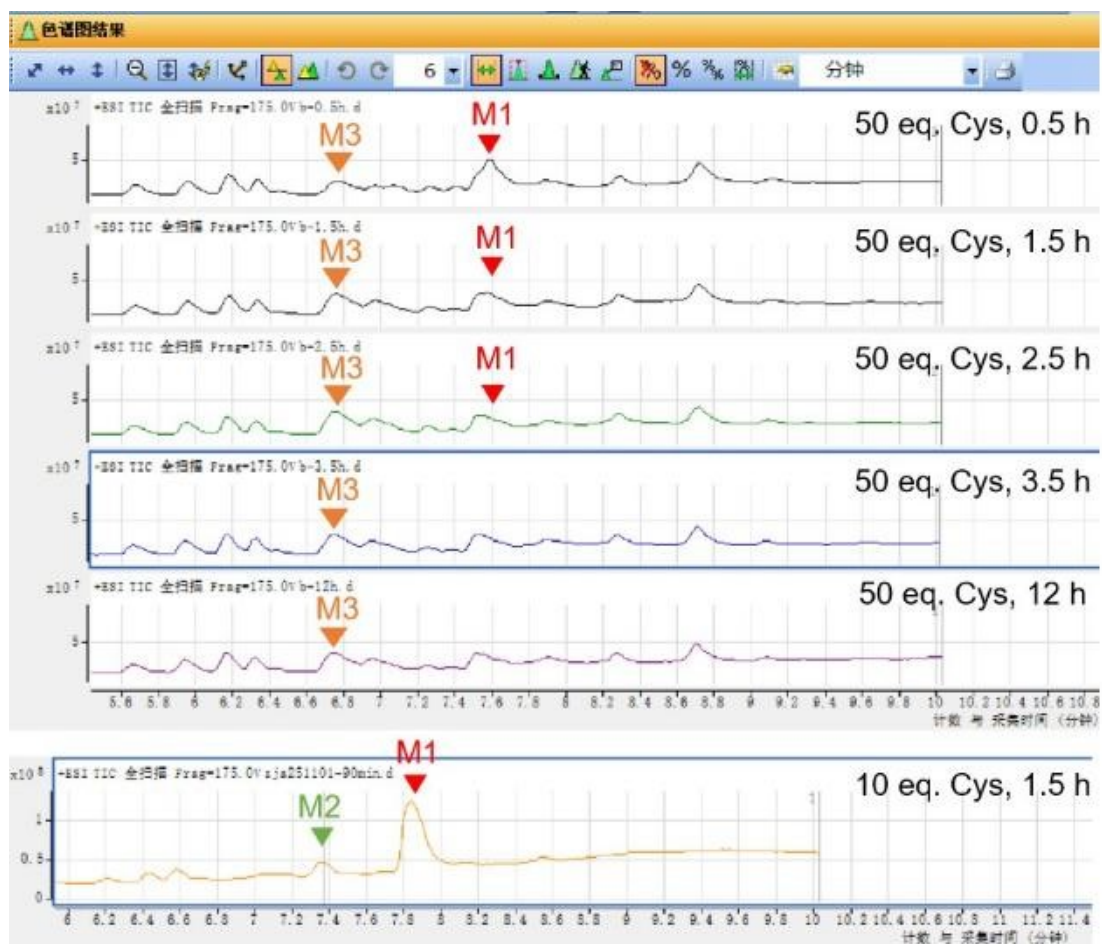


Figure S2. The liquid chromatogram results of B15 of and Cysteine conjugate (M1-M3)

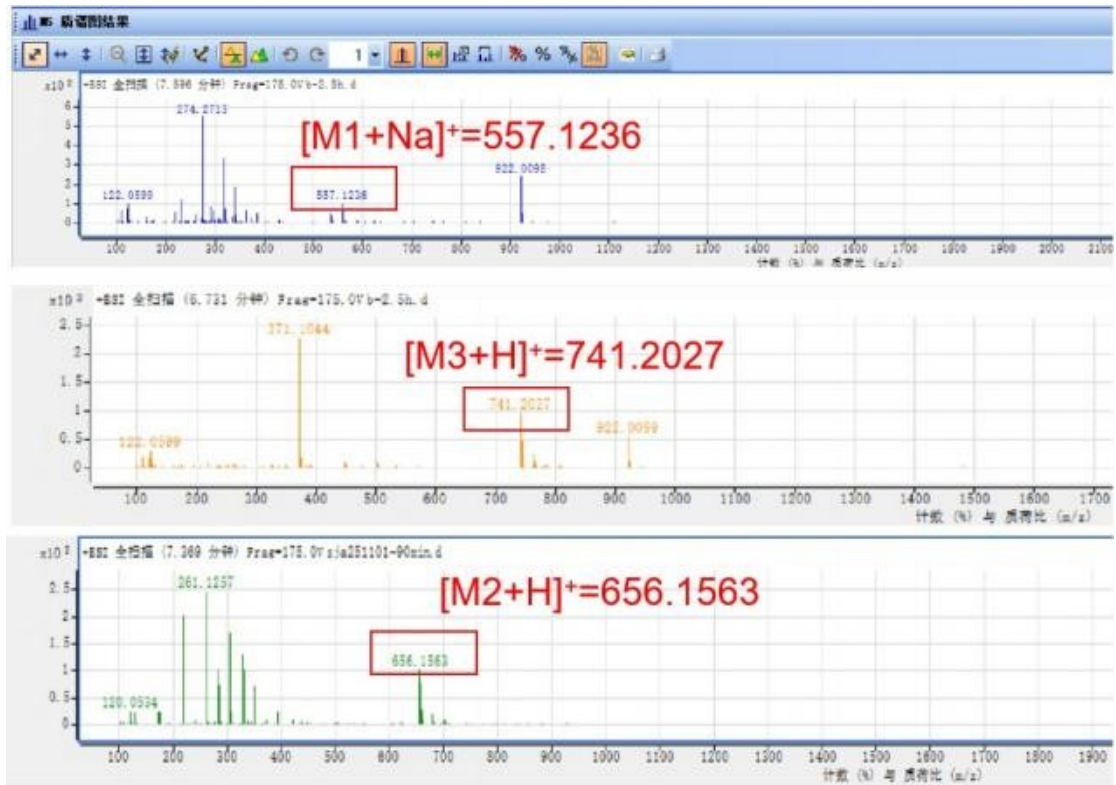


Figure S3. The HRMS spectra of B15 of and Cysteine conjugate (M1-M3)