Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of Quaternary Phosphonium *N*-chloramine Biocides for Antimicrobial Application

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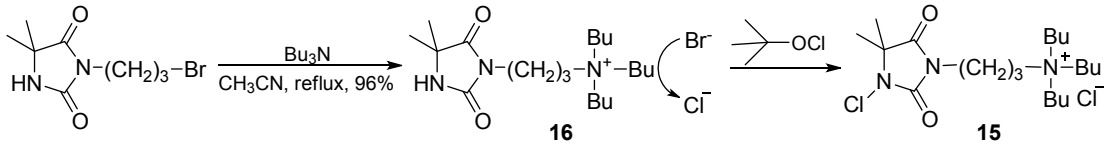
Contents

1. Synthesis protocol of **15** and **16**



Scheme S1 Synthesis route of compound **15**

Synthesis procedure of compound **15** was quite similar to QA *N*-Chloramines **1**, [1] so we herein only present the ^{1}H NMR data of **15** and **16**.

2. NMR spectra analysis of **15** and **16**

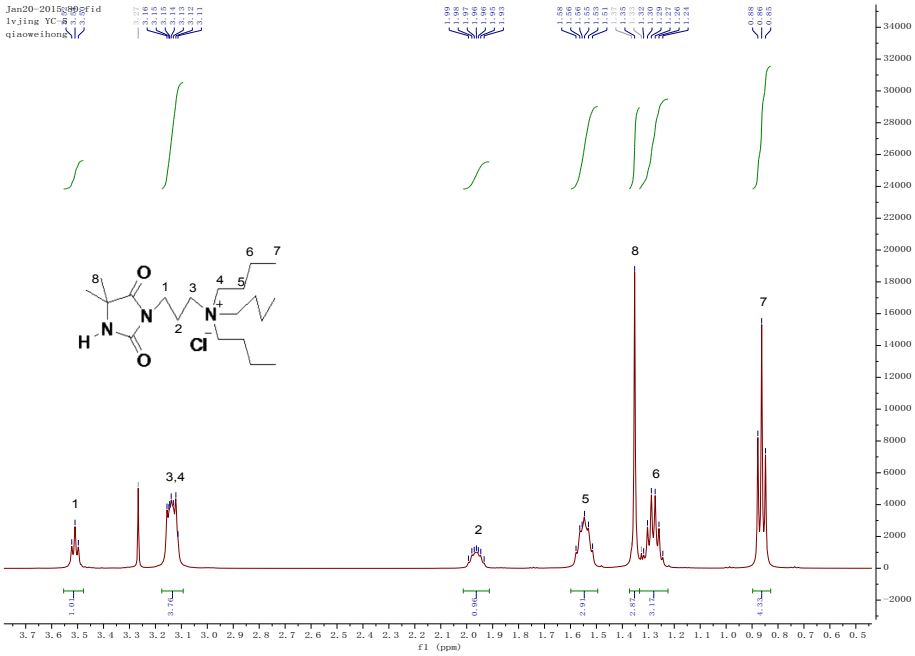


Fig. S1 ^{1}H NMR spectra of compound **16**

Compound **16** ^{1}H NMR (D_2O, 500 MHz, δ) 3.51 (t, J = 6.5 Hz, 2H), 3.09-3.18 (m, 8H), 1.92-2.01 (m, 2H), 1.49-1.60 (m, 6H), 1.35 (s, 6H), 1.22-1.33 (m, 6H), 0.86 (t, J = 7.5 Hz, 9H); ^{13}C NMR (D_2O, 126 MHz, δ) 180.7, 157.0, 59.3, 58.5, 55.3, 35.4, 23.6, 23.3, 20.5, 19.1, 12.9.

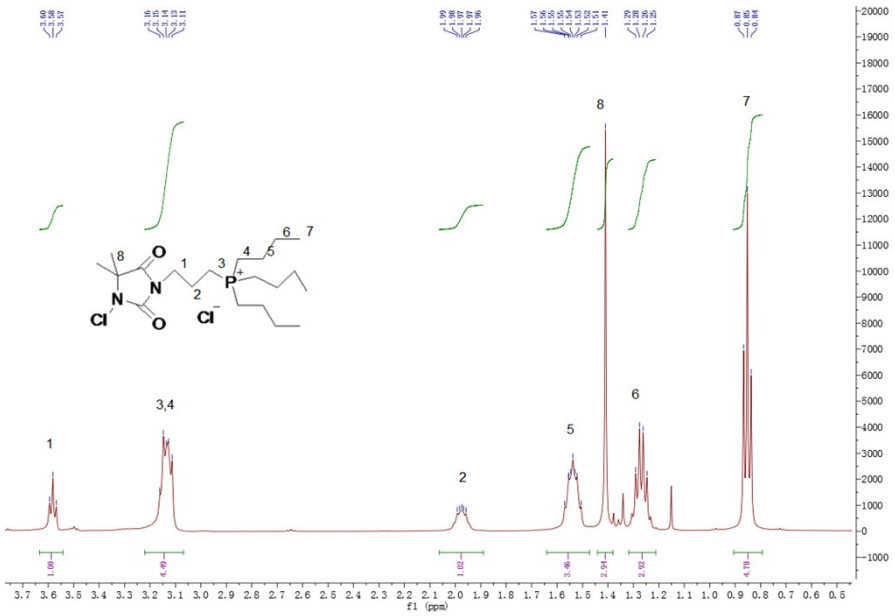


Fig. S2 ^{1}H NMR spectra of compound **15**

Compound **15** ^{1}H NMR (D_2O, 500 MHz, δ) 3.58 (t, *J* = 6.5 Hz, 2H), 3.09-3.19 (m, 8H), 1.93-2.02 (m, 2H), 1.48-1.62 (m, 6H), 1.41 (s, 6H), 1.20-1.39 (m, 6H), 0.85 (t, *J* = 7.5 Hz, 9H); ^{13}C NMR (D_2O, 126 MHz, δ) 176.8, 155.4, 66.4, 58.4, 55.1, 36.6, 232, 21.1, 20.3, 19.1, 12.9.

^{13}C NMR spectra analysis of **5** and **13**

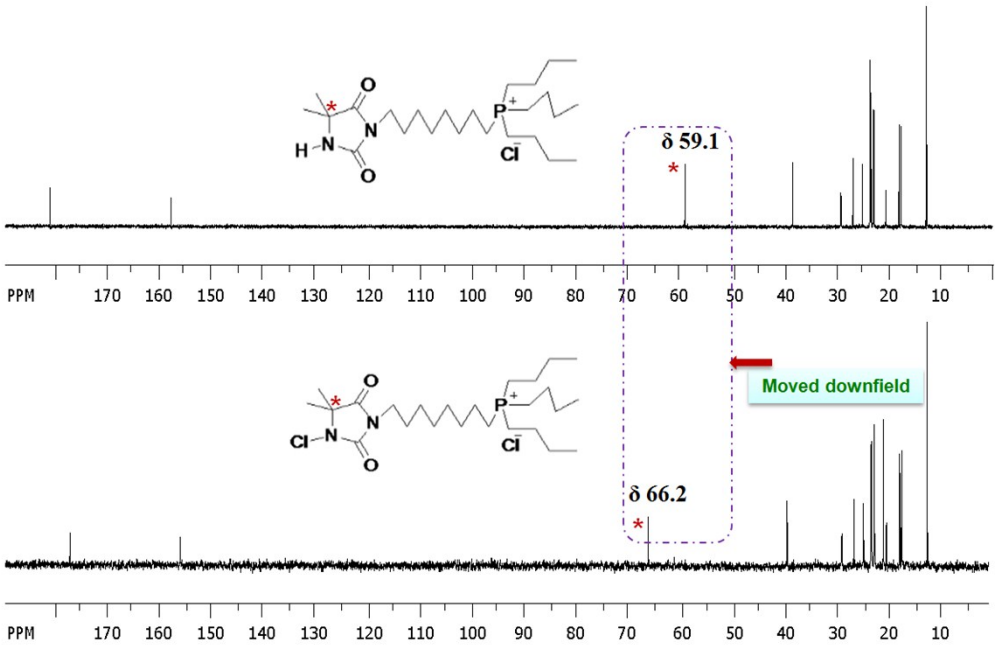
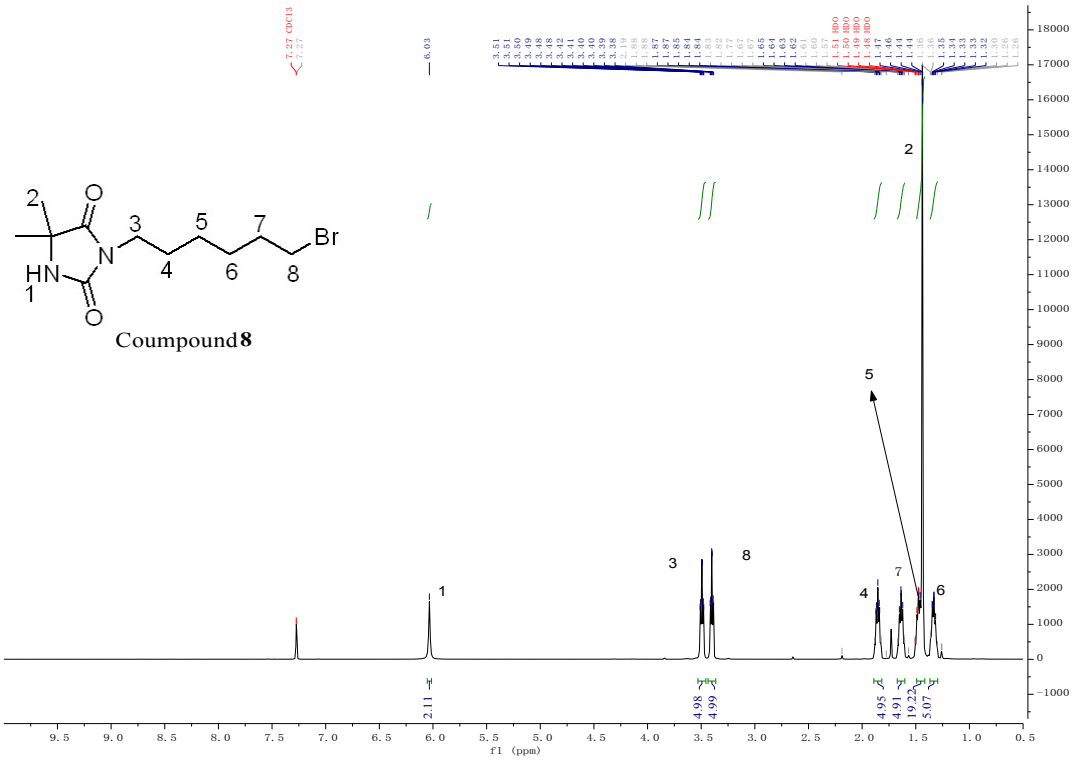


Fig. S3 ^{13}C NMR data of QP *N*-Chloramine **5** and its precursor **13**

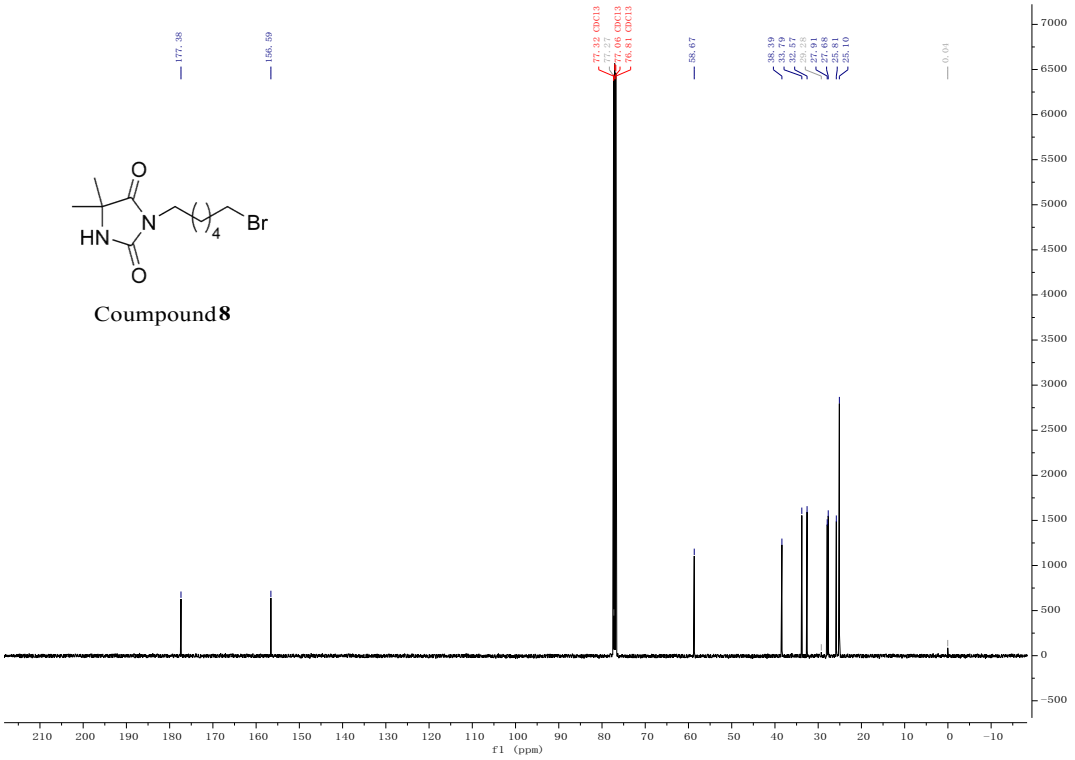
3 References

1. Li, L.; Pu, T.; Zhanel, G.; Zhao, N.; Ens, W.; Liu, S. New biocide with both N-chloramine and quaternary ammonium salt moieties exerts enhanced bactericidal activity. *Adv. Healthcare Mater.* **2012**, *1(5)*, 609-620.

4 Original NMR data



The ^{1}H NMR spectrum of compound **8**



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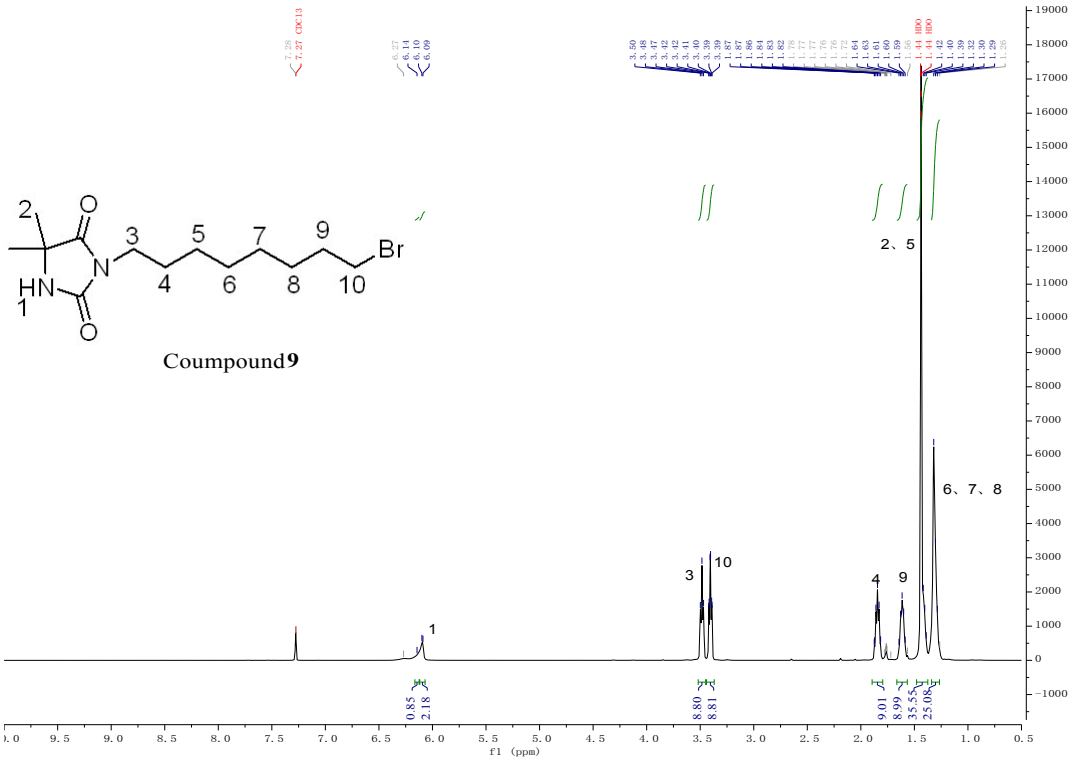
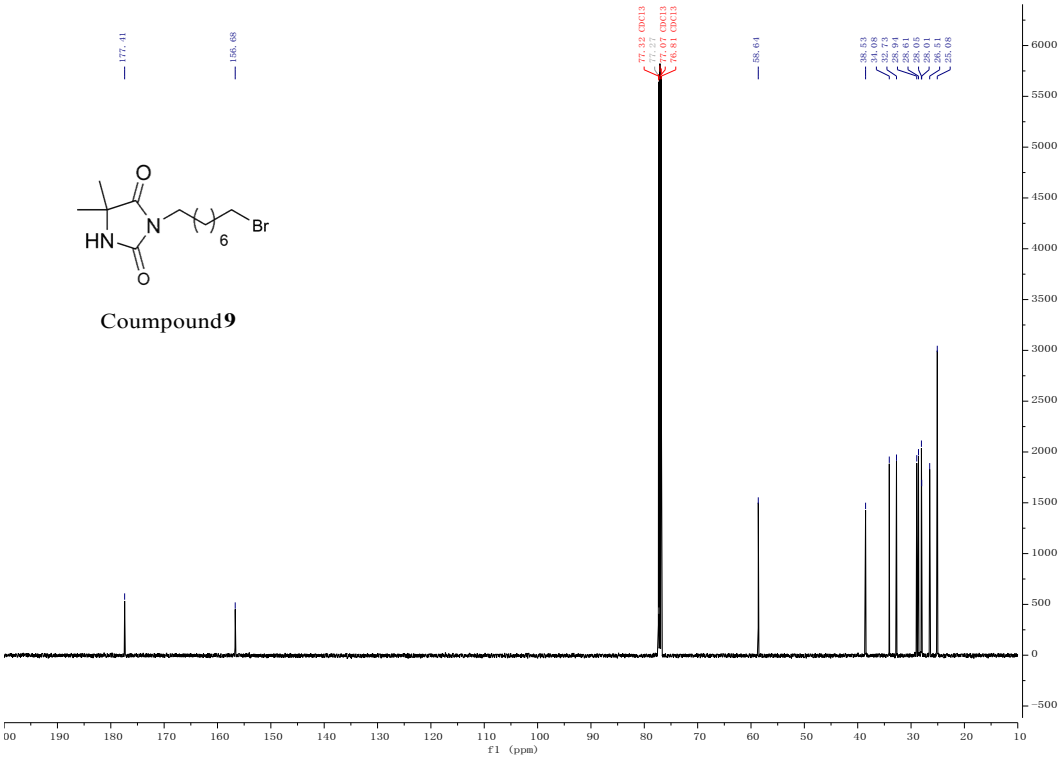


The ^{1}H NMR spectrum of compound **9**



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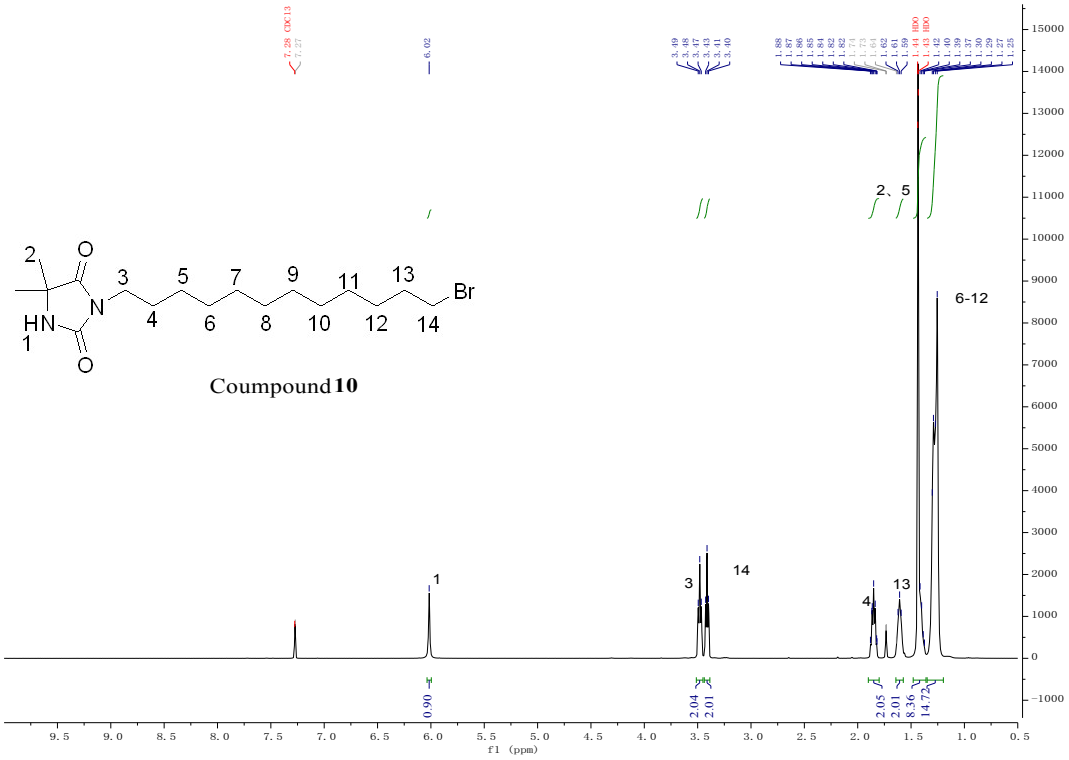

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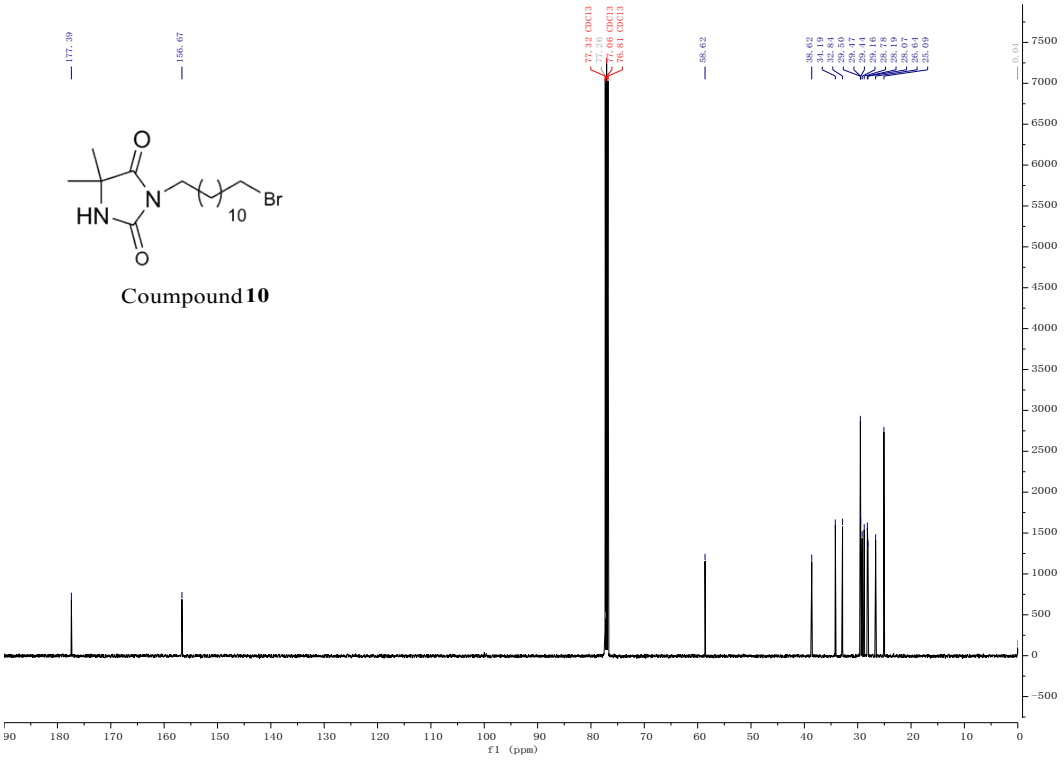
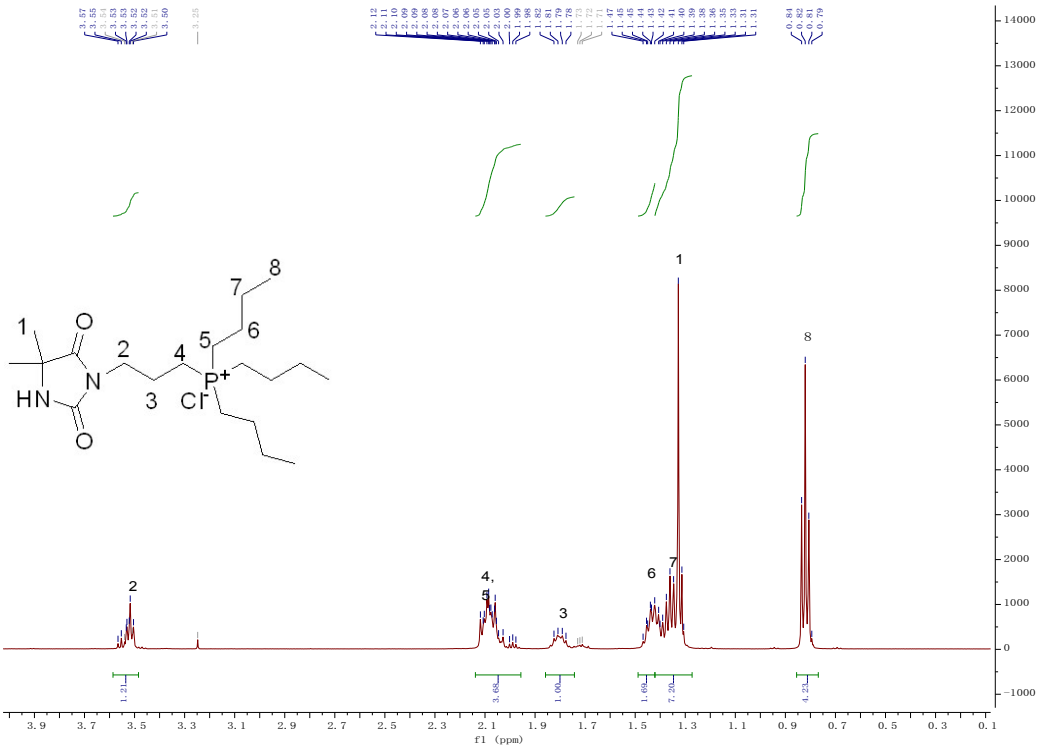


The ^{13}C NMR spectrum of compound **10**



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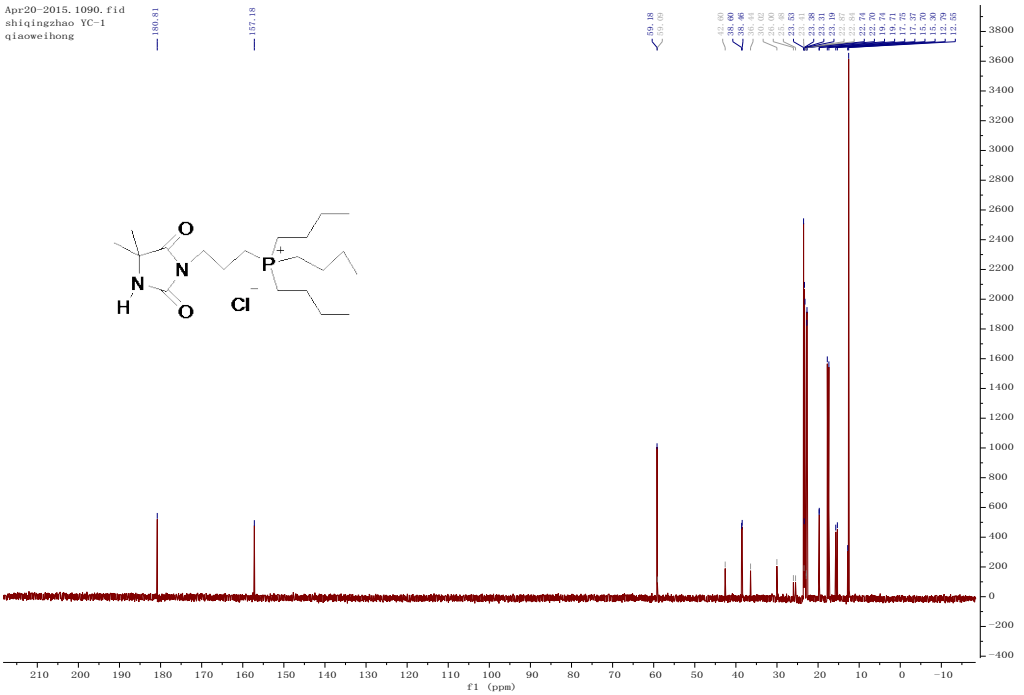

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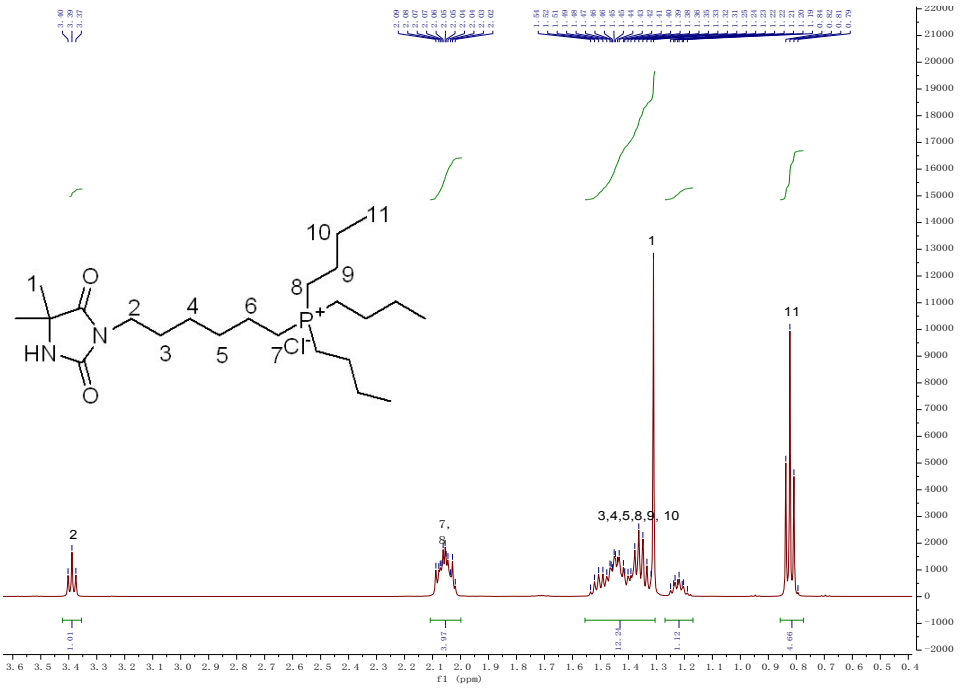

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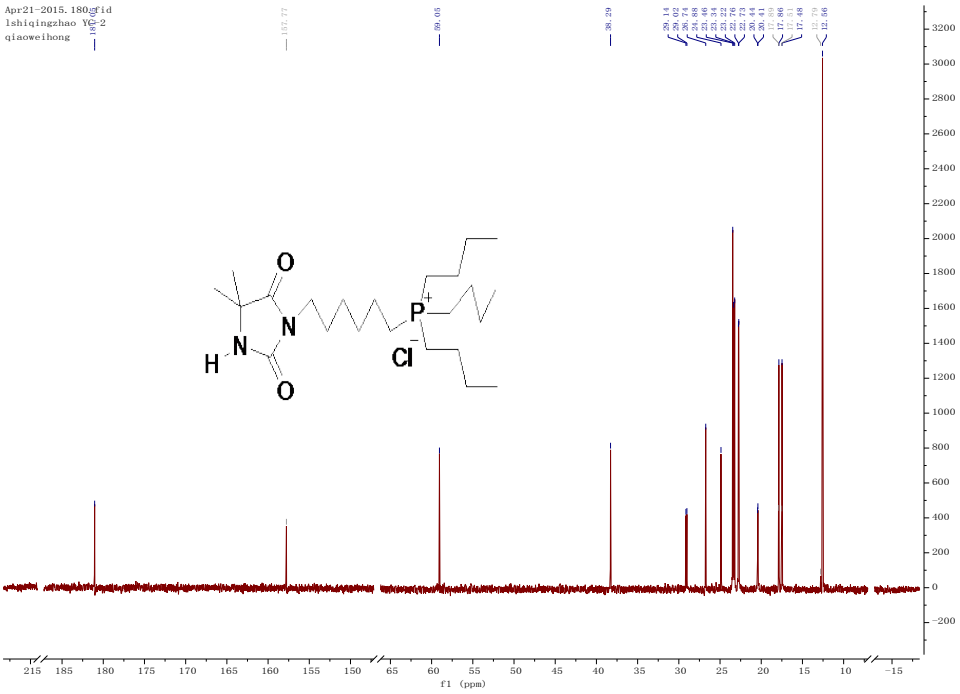

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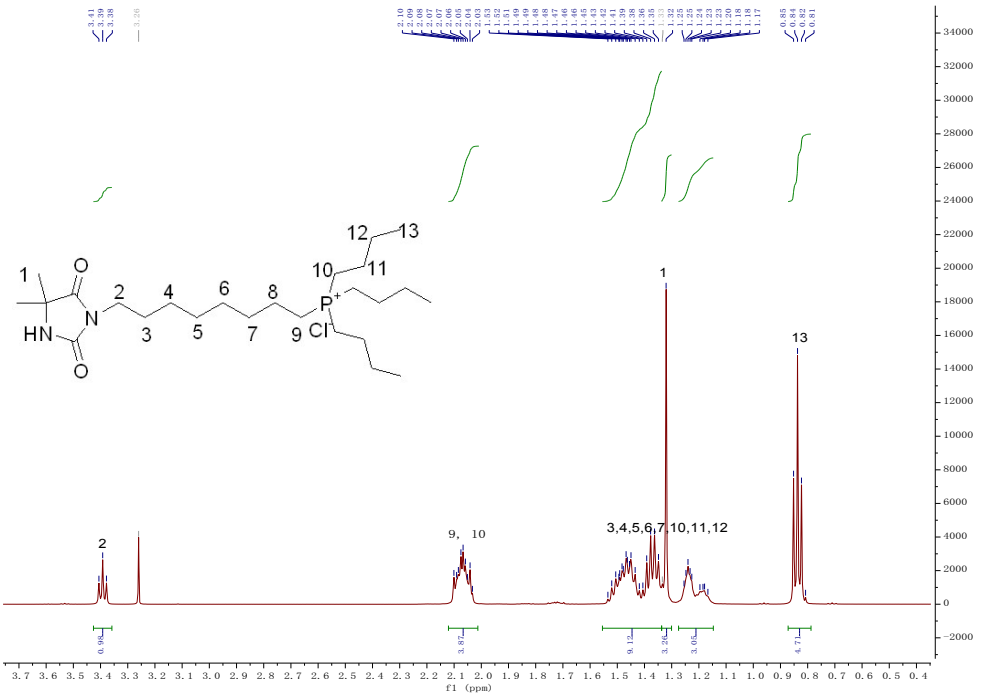

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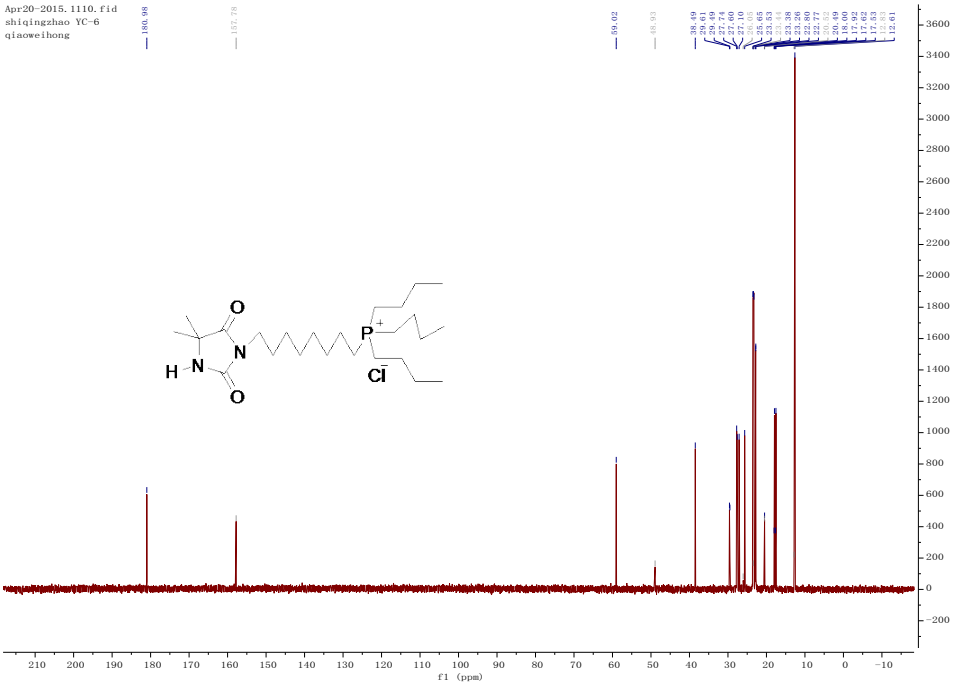

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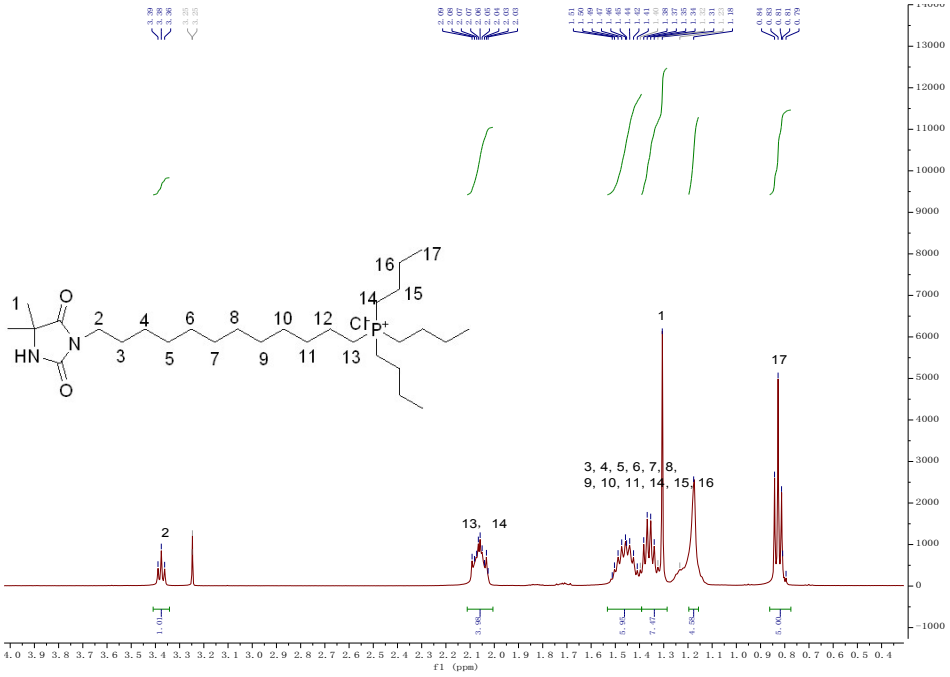

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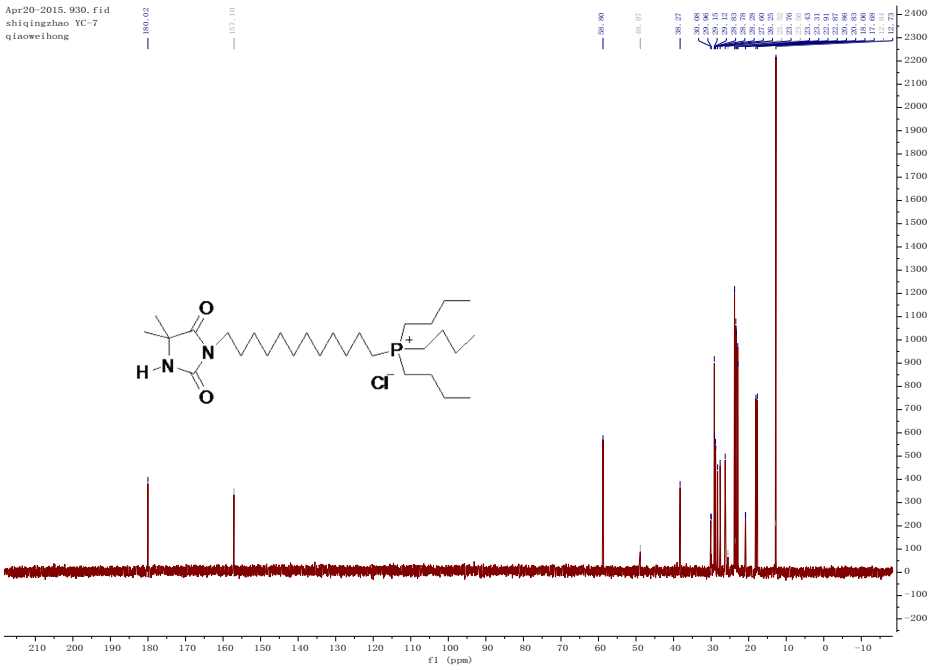

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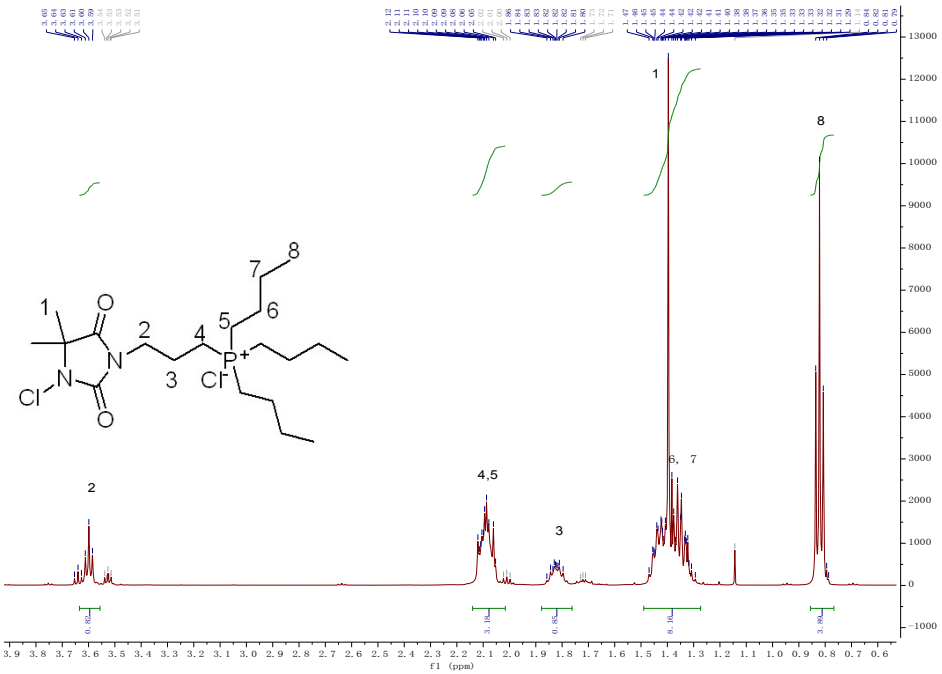

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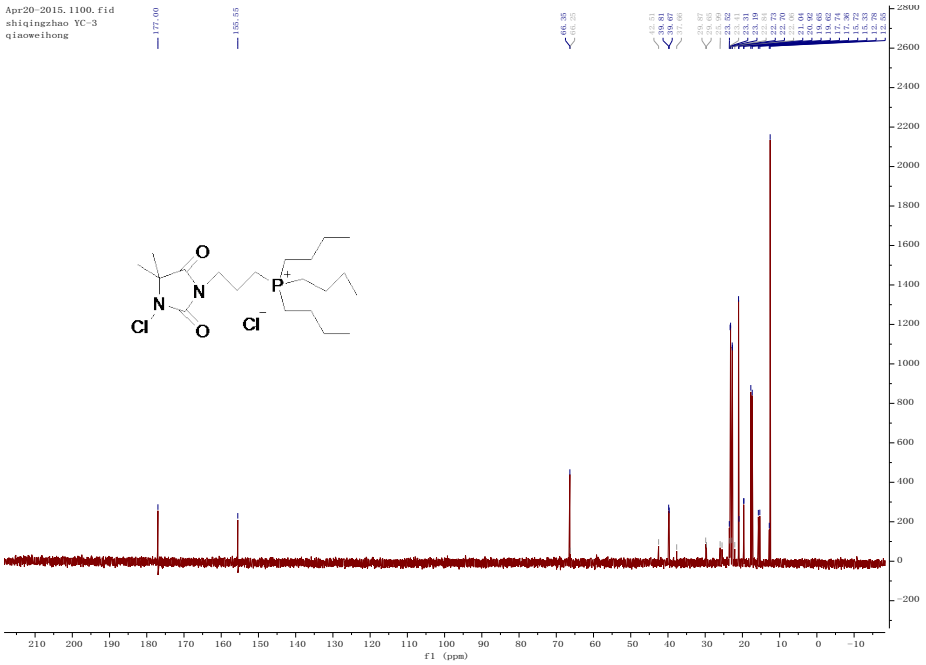

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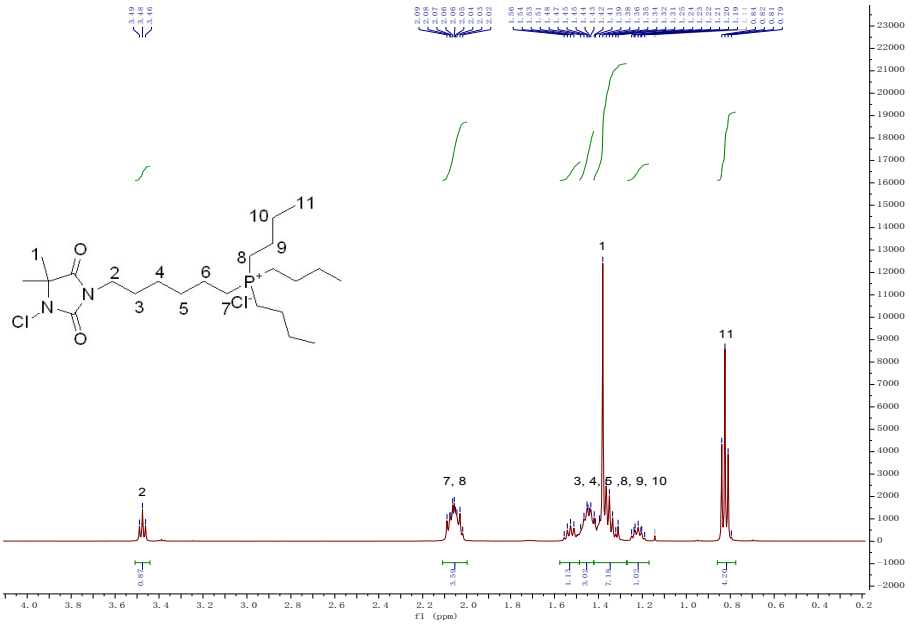

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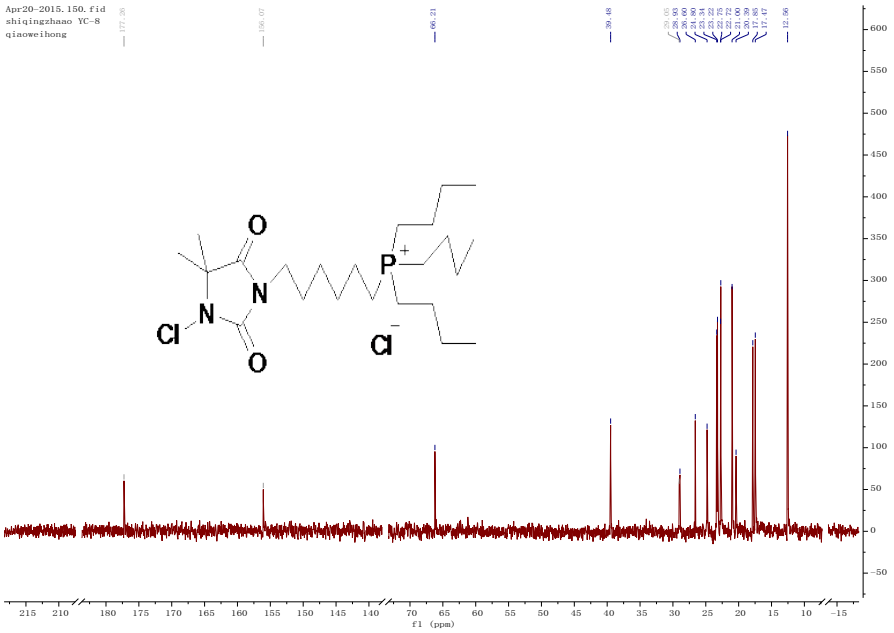

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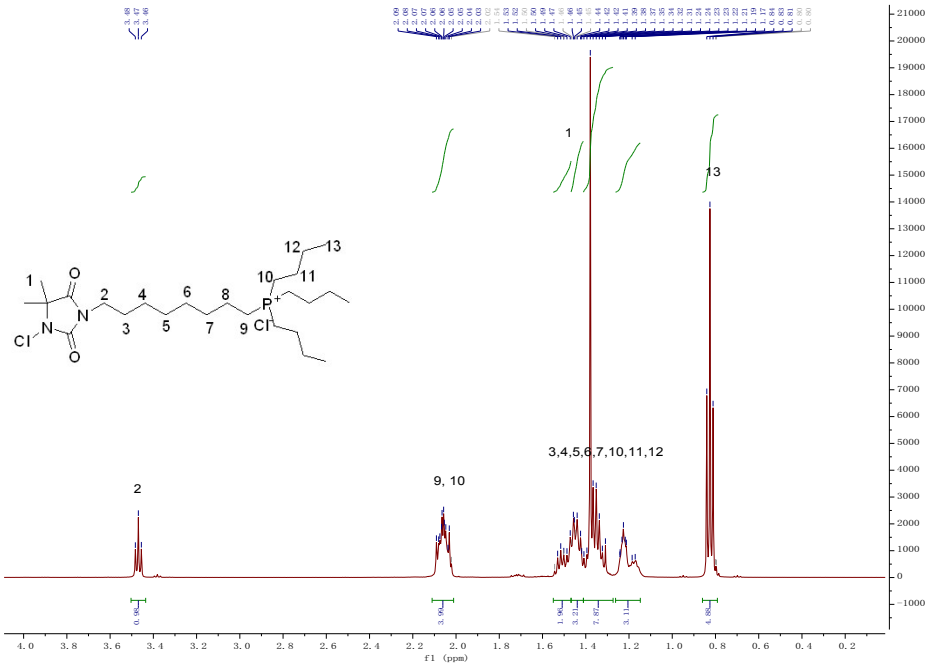

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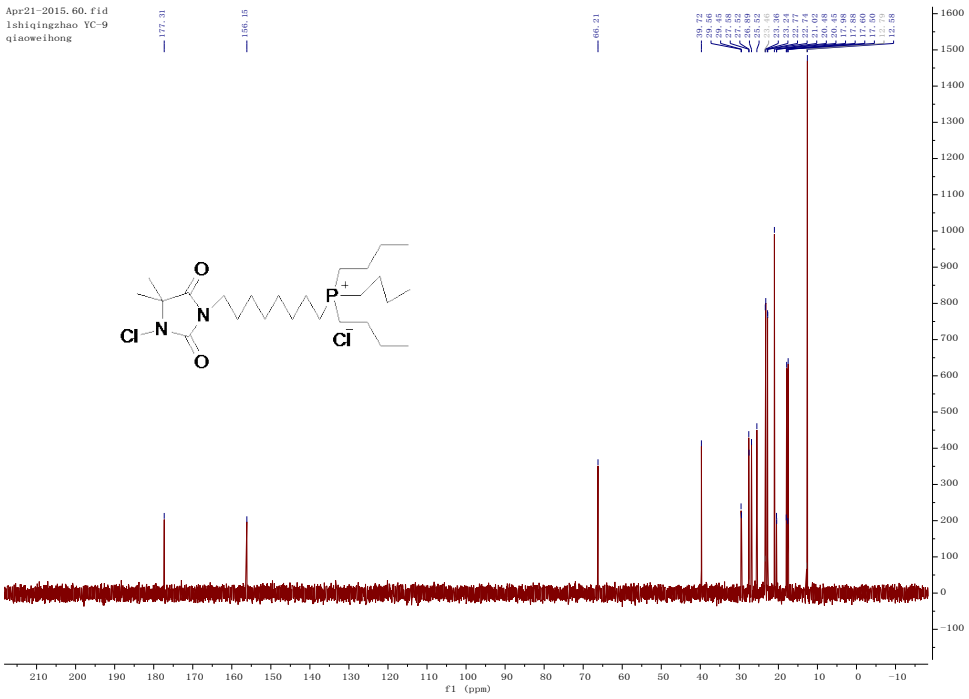

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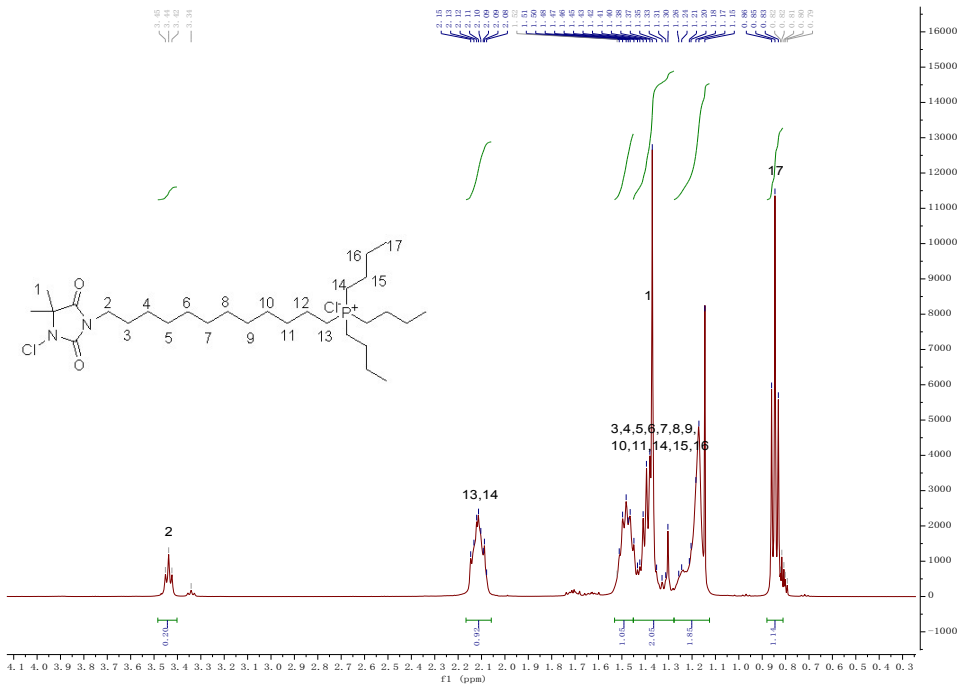

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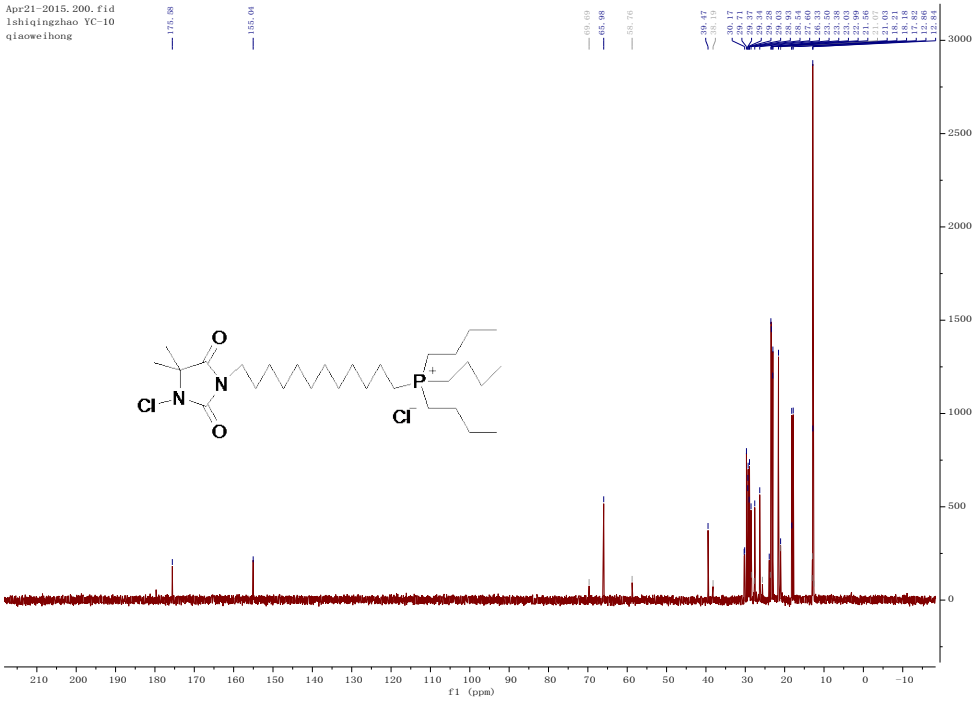

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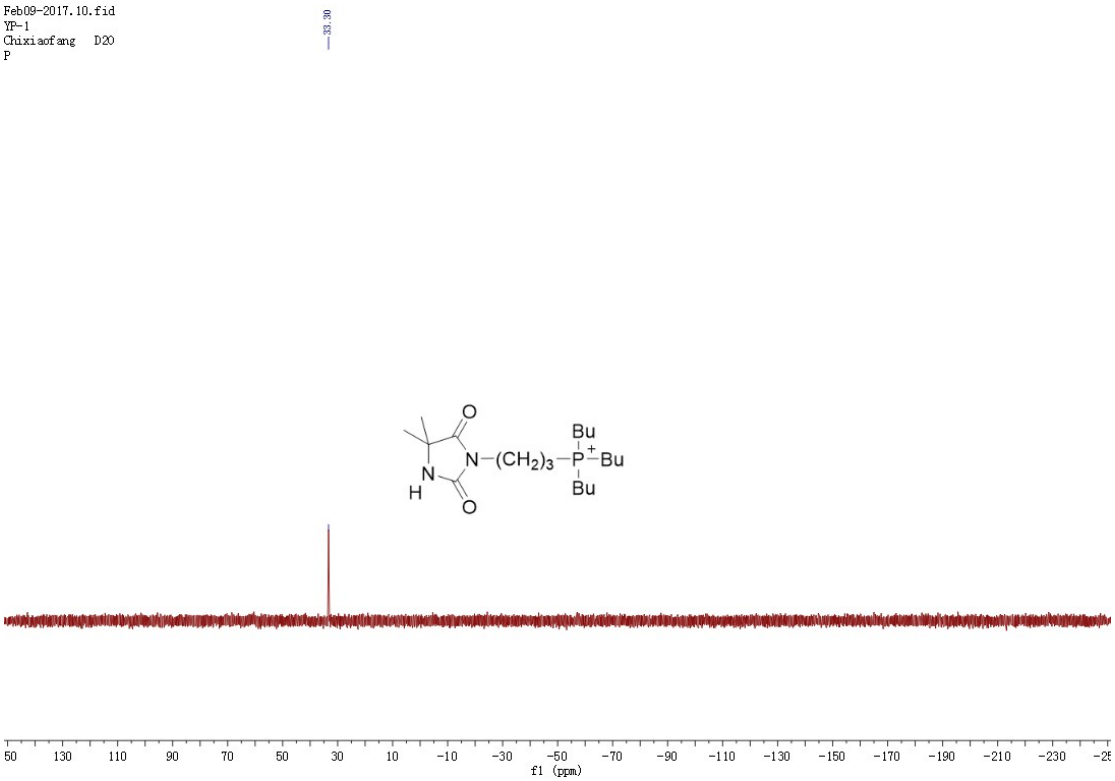

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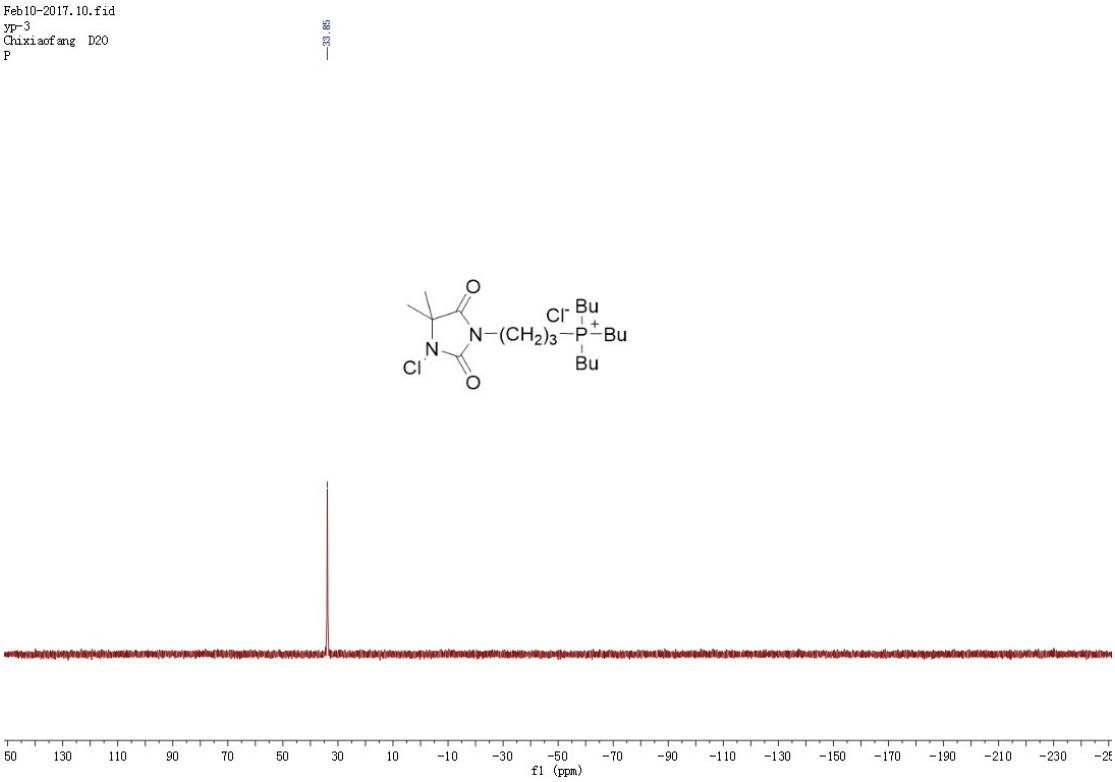

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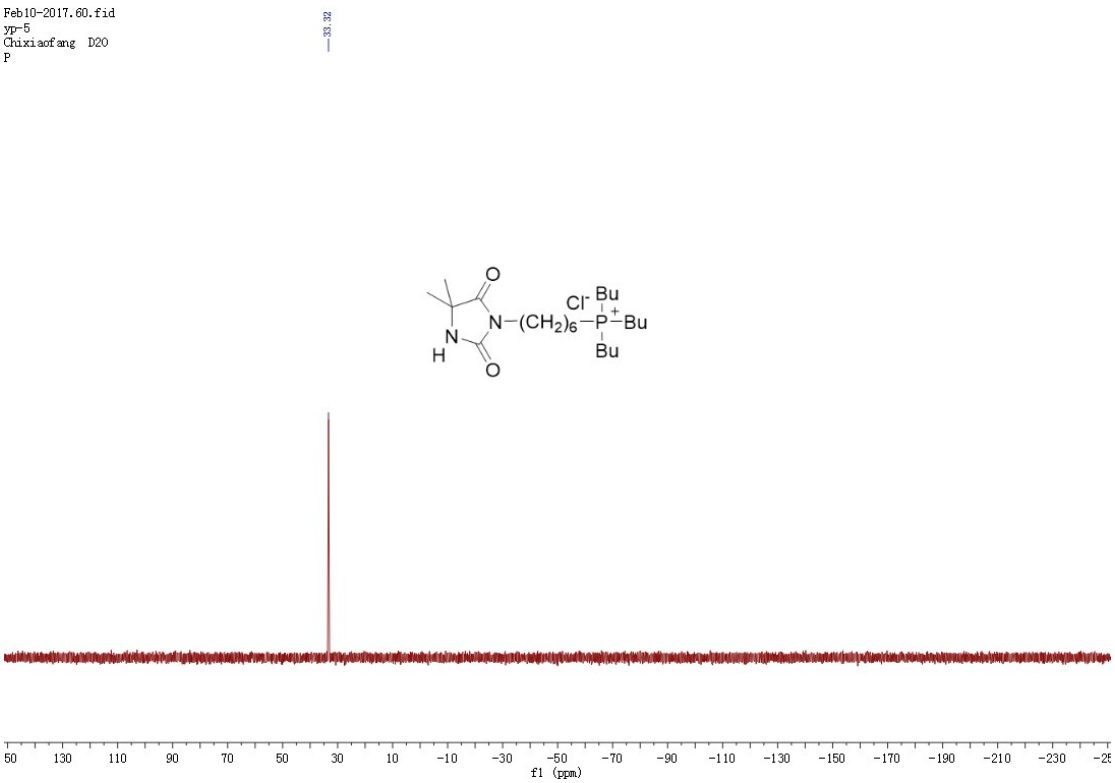

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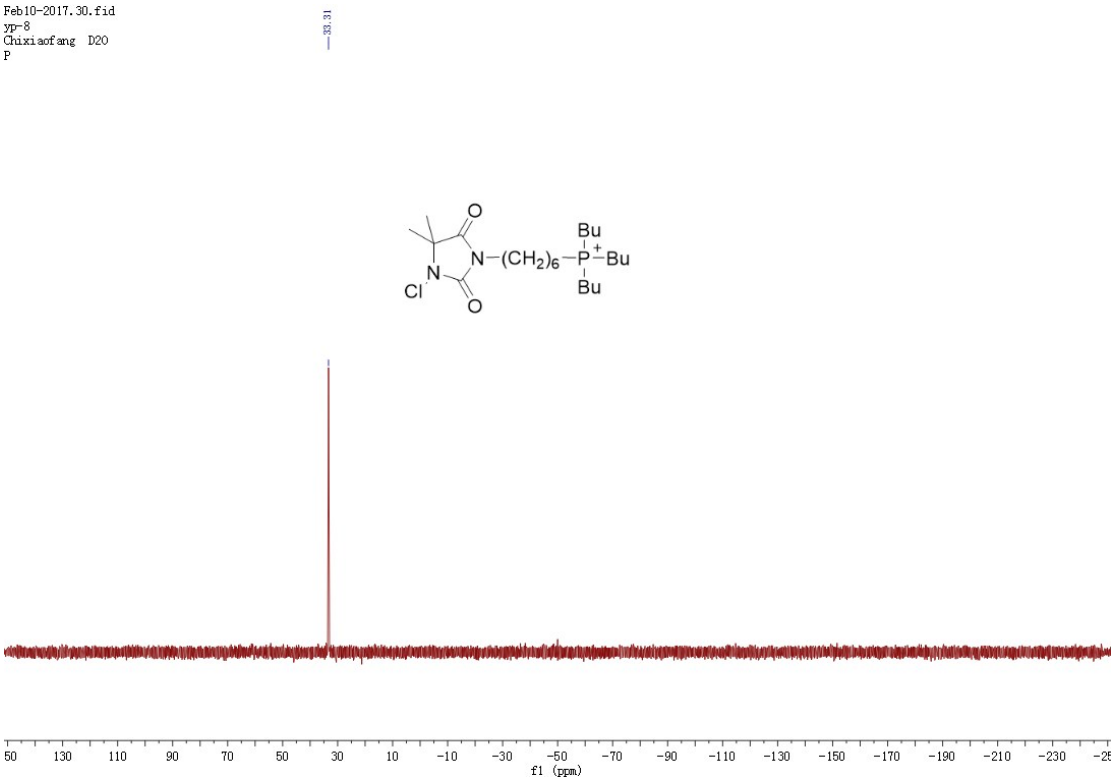

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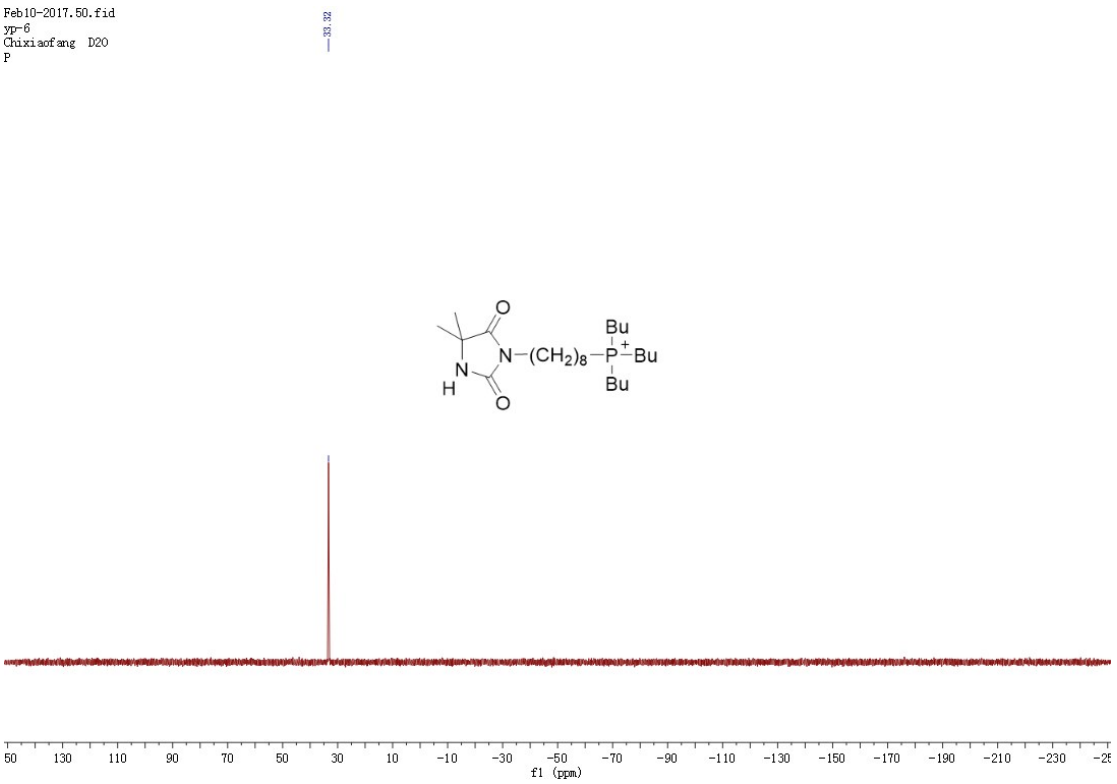

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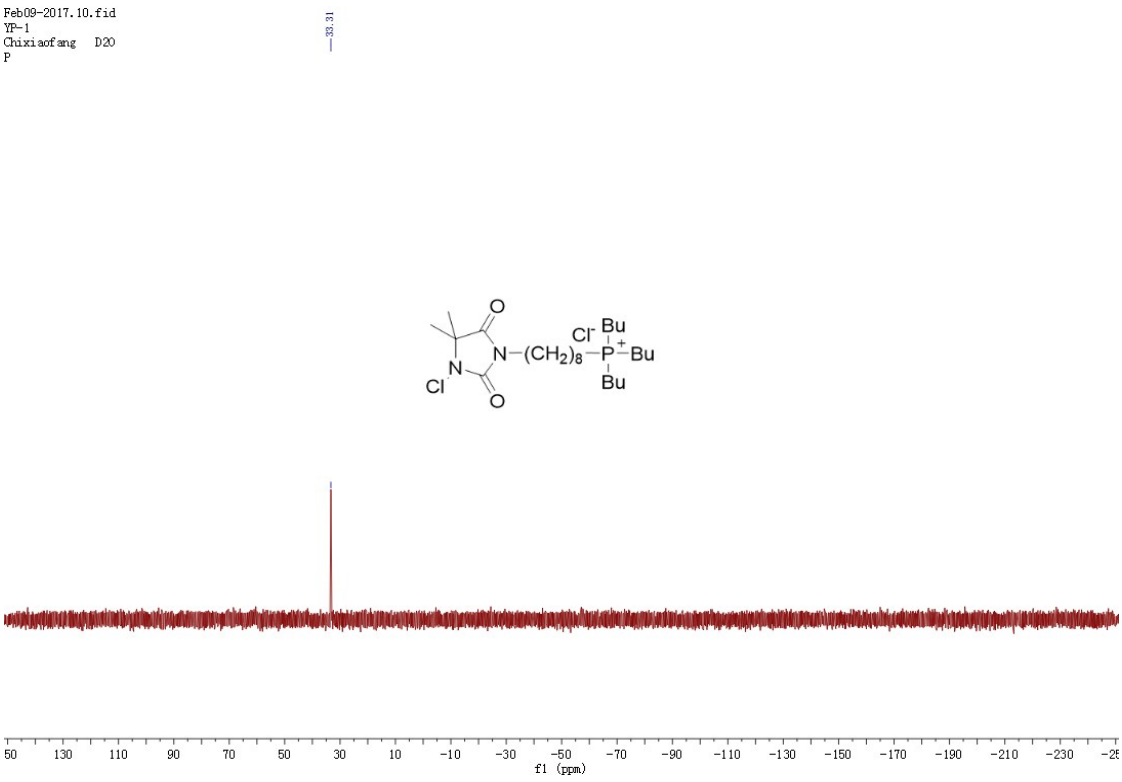

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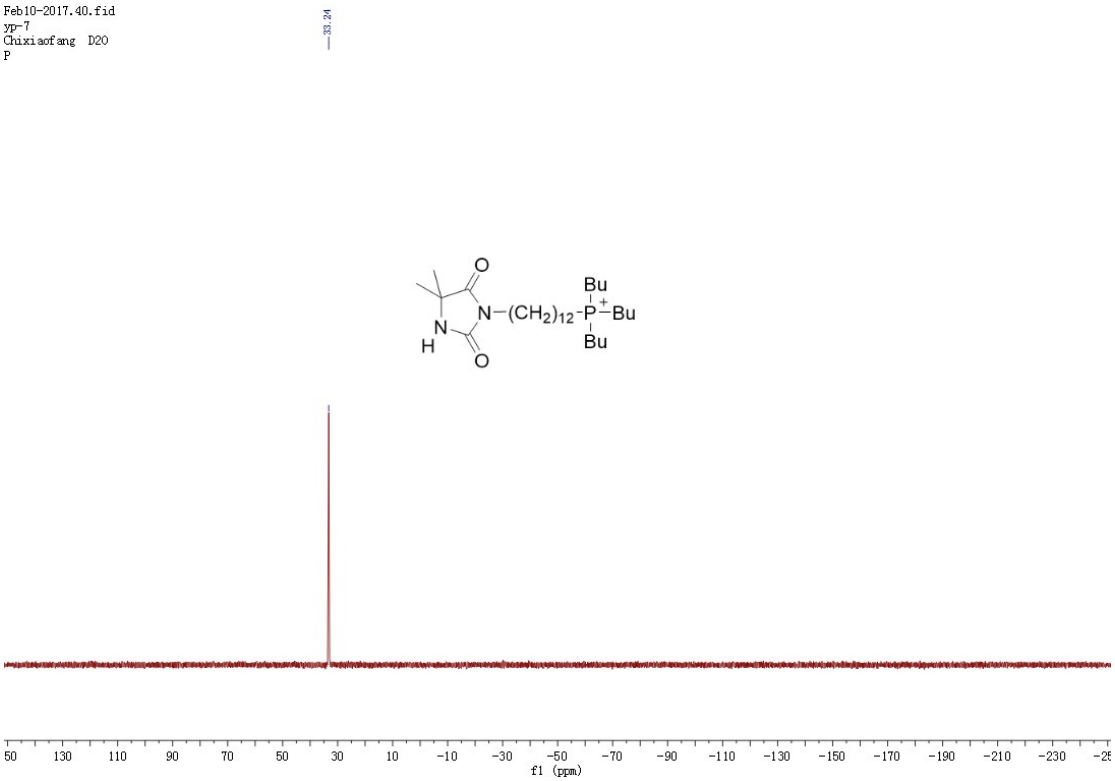

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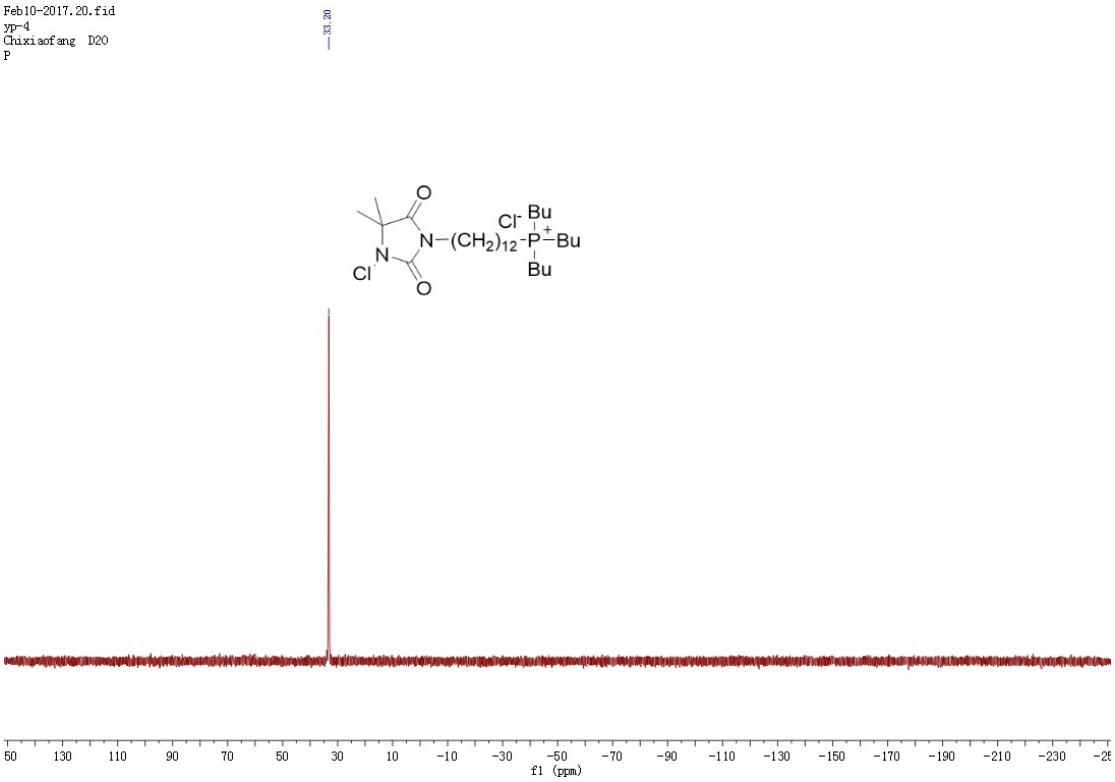

The ^{31}P NMR of compound **6**