

Electronic Supplementary Material

Discovery of cryptolepine derivatives as novel promising agents against phytopathogenic bacteria

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(✉)^{1,2,3}

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1. The comparison results from 16S ribosome gene series alignment for bacteria.

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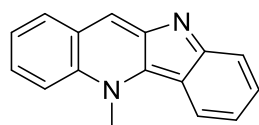
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2. Physical properties of the representative compounds.

¹H NMR, ¹³C NMR and MS of compounds **1-17** and **24** have been reported by our previous work (DOI: 10.1021/acs.jafc.0c06480).

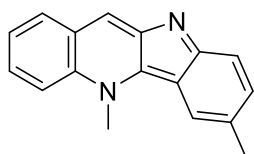
1: 5-methyl-5*H*-indolo[3,2-*b*]quinoline (cryptolepine)



Yield: 34%, purple solid. ¹H NMR (400 MHz, DMSO-*d*₆) δ : 8.90 (s, 1H), 8.47 (dd, *J*

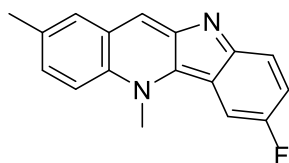
= 11.7, 8.7 Hz, 2H), 8.37 (dd, $J = 8.3, 1.5$ Hz, 1H), 7.87 (t, $J = 8.7$ Hz, 1H), 7.66 (t, $J = 8.0$ Hz, 2H), 7.51 (t, $J = 8.3$ Hz, 1H), 7.05 – 6.97 (m, 1H), 4.89 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ : 160.9, 145.2, 139.4, 133.1, 130.6, 130.0, 129.2, 126.6, 125.4, 124.8, 124.1, 119.8, 116.8, 116.7, 114.1, 39.2. MS-ESI m/z : calcd for $\text{C}_{16}\text{H}_{12}\text{N}_2$ $[\text{M}+\text{H}]^+$: 233.1072; found: 233.2218.

9: 5,7-dimethyl-5H-indolo[3,2-*b*]quinoline



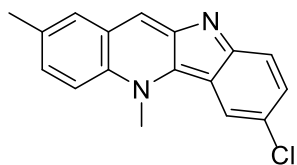
Yield: 21%, purple solid. ^1H NMR (400 MHz, DMSO- d_6) δ : 8.90 (s, 1H), 8.50 (d, $J = 9.0$ Hz, 1H), 8.38 (d, $J = 8.2$ Hz, 1H), 8.25 (s, 1H), 7.91 (t, $J = 7.9$ Hz, 1H), 7.69 (t, $J = 7.5$ Hz, 1H), 7.58 (d, $J = 8.7$ Hz, 1H), 7.40 (d, $J = 8.7$ Hz, 1H), 4.88 (s, 3H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ : 157.6, 143.6, 138.6, 133.6, 133.4, 130.0, 129.6, 126.2, 126.1, 124.8, 124.4, 124.1, 118.6, 117.1, 113.9, 39.3, 21.8. MS-ESI m/z : calcd for $\text{C}_{17}\text{H}_{14}\text{N}_2$ $[\text{M}+\text{H}]^+$: 247.1157; found: 247.0727.

18: 7-fluoro-2,5-dimethyl-5H-indolo[3,2-*b*]quinoline



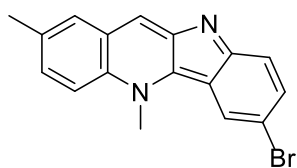
Yield: 18%, purple solid. ^1H NMR (400 MHz, DMSO- d_6) δ : 8.86 (s, 1H), 8.52 – 8.07 (m, 3H), 7.86 – 7.60 (m, 2H), 7.52 – 7.44 (m, 1H), 4.83 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ : 155.5, 145.5, 138.3, 133.4, 131.9, 128.5, 127.1, 125.2, 124.1, 120.9, 120.4, 120.0, 116.7, 112.2, 108.7, 39.1, 21.1. MS-ESI m/z : calcd for $\text{C}_{17}\text{H}_{13}\text{FN}_2$ $[\text{M}+\text{H}]^+$: 265.1136; found: 265.1421.

19: 7-chloro-2,5-dimethyl-5H-indolo[3,2-*b*]quinoline



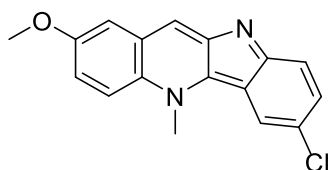
Yield: 17%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.88 (s, 1H), 8.48 (d, $J = 2.1$ Hz, 1H), 8.43 (d, $J = 9.2$ Hz, 1H), 8.13 (s, 1H), 7.75 (dd, $J = 9.2, 2.0$ Hz, 1H), 7.65 (d, $J = 9.1$ Hz, 1H), 7.51 – 7.45 (m, 1H), 4.86 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 157.8, 148.9, 145.4, 133.9, 132.1, 130.4, 128.5, 127.3, 125.2, 123.9, 121.0, 120.7, 116.9, 114.5, 112.2, 39.4, 21.1. MS-ESI m/z : calcd for $\text{C}_{17}\text{H}_{13}\text{ClN}_2$ $[\text{M}+\text{H}]^+$: 281.0840; found: 281.0100.

20: 7-bromo-2,5-dimethyl-5H-indolo[3,2-*b*]quinoline



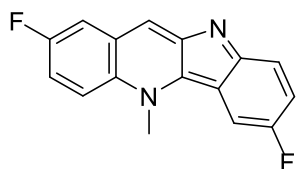
Yield: 22%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.90 (s, 1H), 8.63 (s, 1H), 8.45 (d, $J = 9.1$ Hz, 1H), 8.16 (s, 1H), 7.77 (dd, $J = 9.2, 2.0$ Hz, 1H), 7.64 – 7.56 (m, 2H), 4.87 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 157.7, 145.2, 138.5, 134.0, 132.8, 132.1, 128.6, 127.3, 127.0, 125.3, 121.3, 116.9, 115.3, 112.0, 107.6, 39.4, 21.1. MS-ESI m/z : calcd for $\text{C}_{17}\text{H}_{13}\text{BrN}_2$ $[\text{M}+\text{H}]^+$: 325.0355; found: 324.9641.

21: 7-chloro-2-methoxy-5-methyl-5H-indolo[3,2-*b*]quinoline



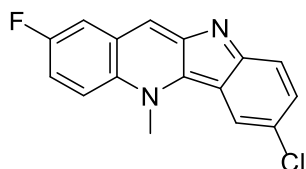
Yield: 17%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.85 (s, 1H), 8.50 – 8.43 (m, 2H), 7.78 (d, $J = 2.8$ Hz, 1H), 7.64 (d, $J = 9.0$ Hz, 1H), 7.56 (dd, $J = 9.7, 2.7$ Hz, 1H), 7.49 (dd, $J = 9.0, 2.0$ Hz, 1H), 4.86 (s, 3H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 155.9, 146.2, 137.3, 133.6, 130.5, 129.6, 126.7, 126.1, 123.8, 122.6, 120.9, 120.3, 118.8, 114.6, 107.3, 56.1, 39.6. MS-ESI m/z : calcd for $\text{C}_{17}\text{H}_{13}\text{ClN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 297.0789; found: 297.0209.

22: 2,7-difluoro-5-methyl-5H-indolo[3,2-*b*]quinoline uinoline



Yield: 32%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.93 (s, 1H), 8.61 (dd, $J = 9.8, 4.7$ Hz, 1H), 8.32 – 8.25 (m, 1H), 8.21 (dd, $J = 9.5, 2.9$ Hz, 1H), 7.85 – 7.79 (m, 1H), 7.69 (dd, $J = 9.3, 5.0$ Hz, 1H), 7.53 – 7.44 (m, 1H), 4.89 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 158.1, 146.5, 138.7, 134.4, 130.3, 126.7, 125.5, 120.9, 120.7, 120.0, 119.2, 118.9, 112.6, 112.4, 109.0, 39.4. MS-ESI m/z : calcd for $\text{C}_{16}\text{H}_{10}\text{F}_2\text{N}_2$ $[\text{M}+\text{H}]^+$: 269.0885; found: 269.1165.

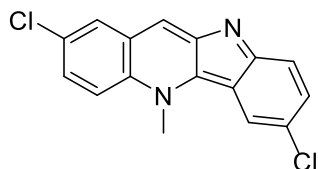
23: 7-chloro-2-fluoro-5-methyl-5H-indolo[3,2-*b*]quinoline



Yield: 34%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.97 (s, 1H), 8.65 (dd, $J = 9.9, 4.6$ Hz, 1H), 8.54 (d, $J = 2.1$ Hz, 1H), 8.24 (dd, $J = 9.5, 3.0$ Hz, 1H), 7.89 – 7.80 (m, 1H), 7.69 (d, $J = 9.1$ Hz, 1H), 7.53 (dd, $J = 9.0, 2.1$ Hz, 1H), 4.93 (s, 3H).

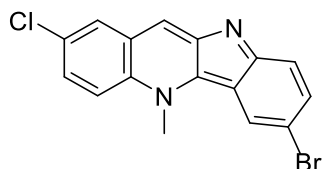
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 158.2, 146.4, 142.6, 138.9, 135.0, 131.0, 130.5, 127.2, 125.8, 124.1, 121.3, 120.8, 120.2, 114.4, 112.4, 39.4. MS-ESI m/z : calcd for $\text{C}_{16}\text{H}_{10}\text{ClFN}_2$ $[\text{M}+\text{H}]^+$: 285.0589; found: 285.0162.

25: 2,7-dichloro-5-methyl-5H-indolo[3,2-*b*]quinoline



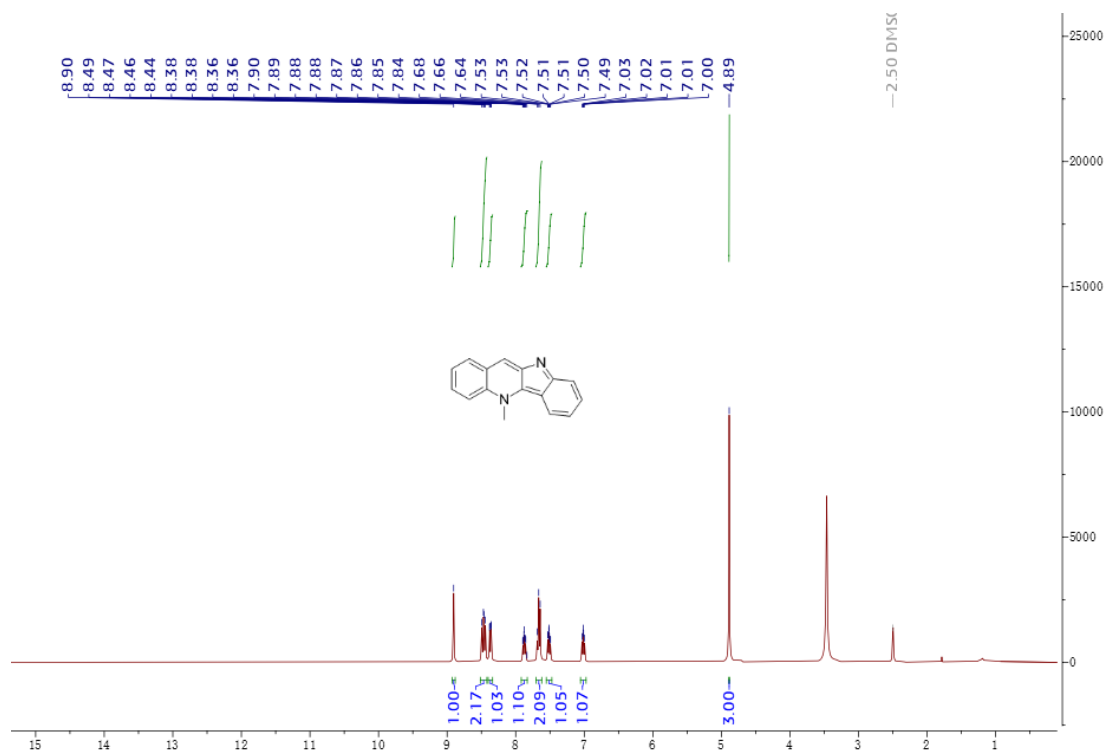
Yield: 37%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.97 (s, 1H), 8.63 – 8.50 (m, 3H), 7.90 (dd, $J = 9.6, 2.5$ Hz, 1H), 7.69 (d, $J = 9.2$ Hz, 1H), 7.52 (dd, $J = 9.2, 2.2$ Hz, 1H), 4.90 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 159.4, 153.5, 147.3, 139.0, 136.5, 133.4, 131.1, 129.4, 126.8, 125.9, 124.1, 121.4, 119.5, 114.5, 105.4, 39.3. MS-ESI m/z : calcd for $\text{C}_{16}\text{H}_{10}\text{Cl}_2\text{N}_2$ $[\text{M}+\text{H}]^+$: 301.0294; found: 300.9716.

26: 7-bromo-2-chloro-5-methyl-5H-indolo[3,2-*b*]quinoline

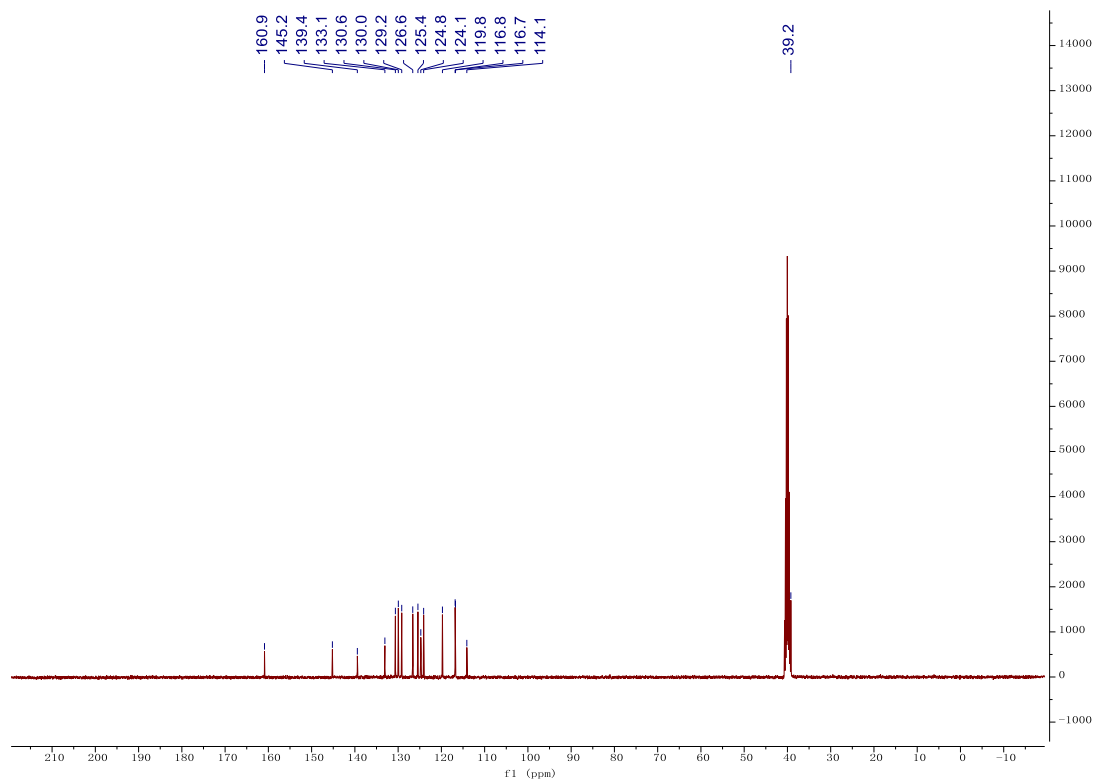


Yield: 36%, purple solid. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ : 8.96 (s, 1H), 8.64 (s, 1H), 8.59 (d, $J = 9.6$ Hz, 1H), 8.54 (d, $J = 2.4$ Hz, 1H), 7.90 (dd, $J = 9.5, 2.5$ Hz, 1H), 7.67 – 7.55 (m, 2H), 4.89 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ : 159.32, 146.11, 138.88, 133.41, 131.83, 129.43, 128.64, 128.19, 127.21, 126.84, 125.72, 121.82, 119.51, 115.36, 108.86, 39.38. MS-ESI m/z : calcd for $\text{C}_{16}\text{H}_{10}\text{BrClN}_2$ $[\text{M}+\text{H}]^+$: 346.9768; found: 346.9276.

3. Spectrums of the representative compounds.



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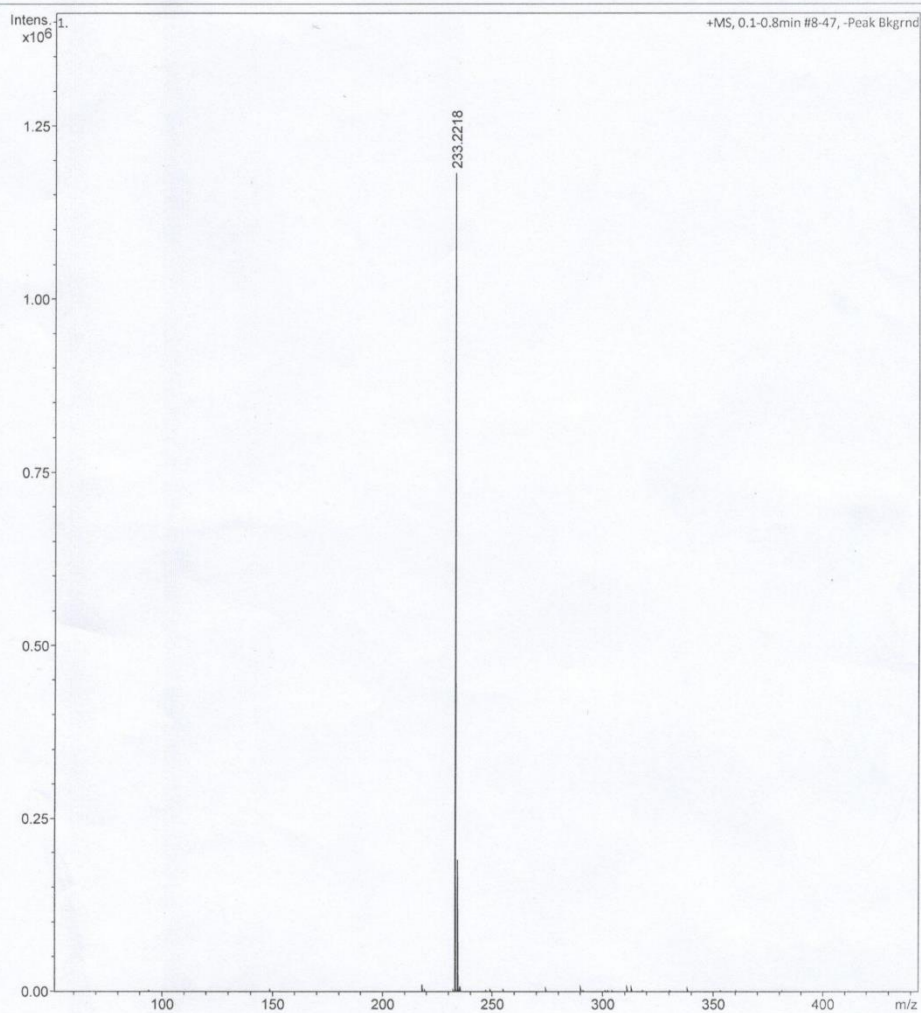


The ^{13}C NMR spectrum of compound 1

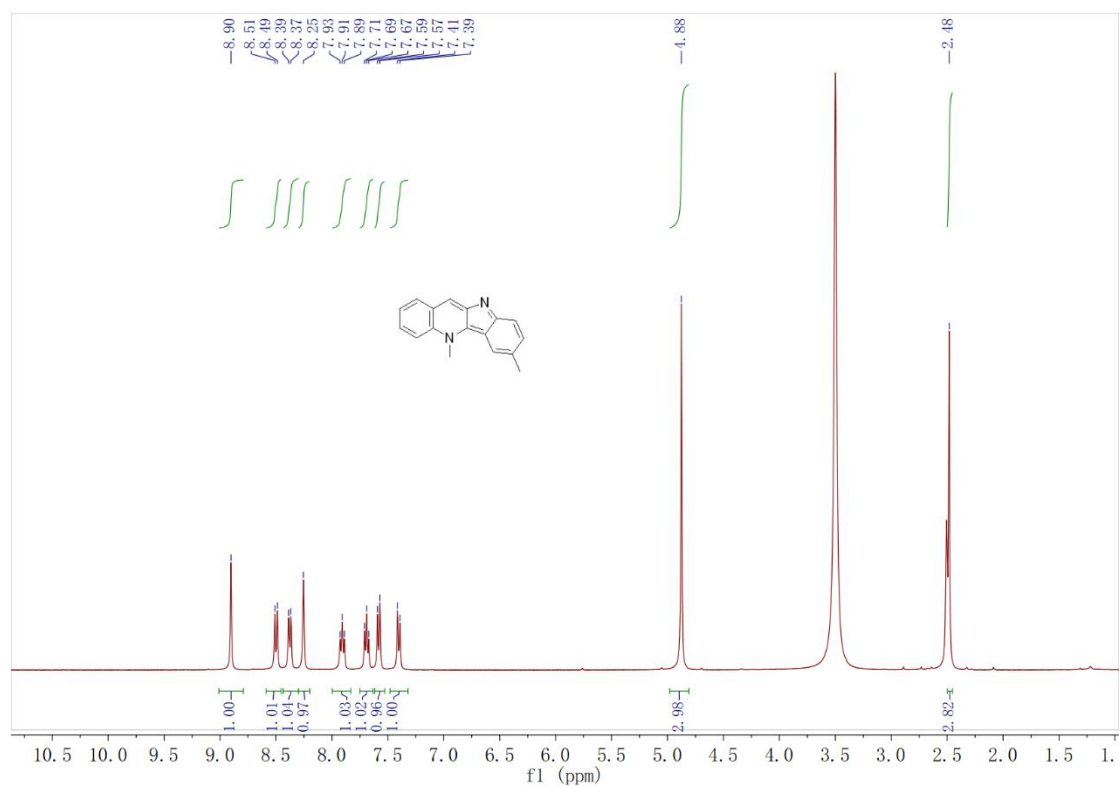
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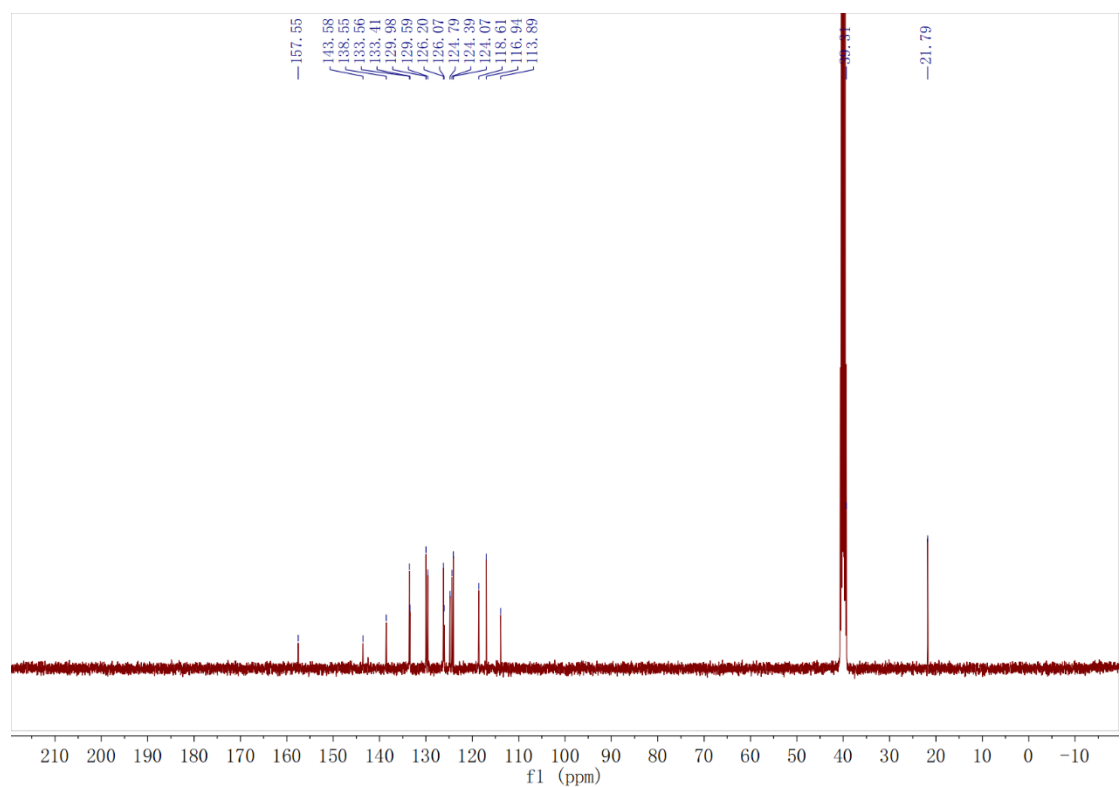
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The Mass spectrogram of compound 1



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



The ^{13}C NMR spectrum of compound **9**

Generic Display Report

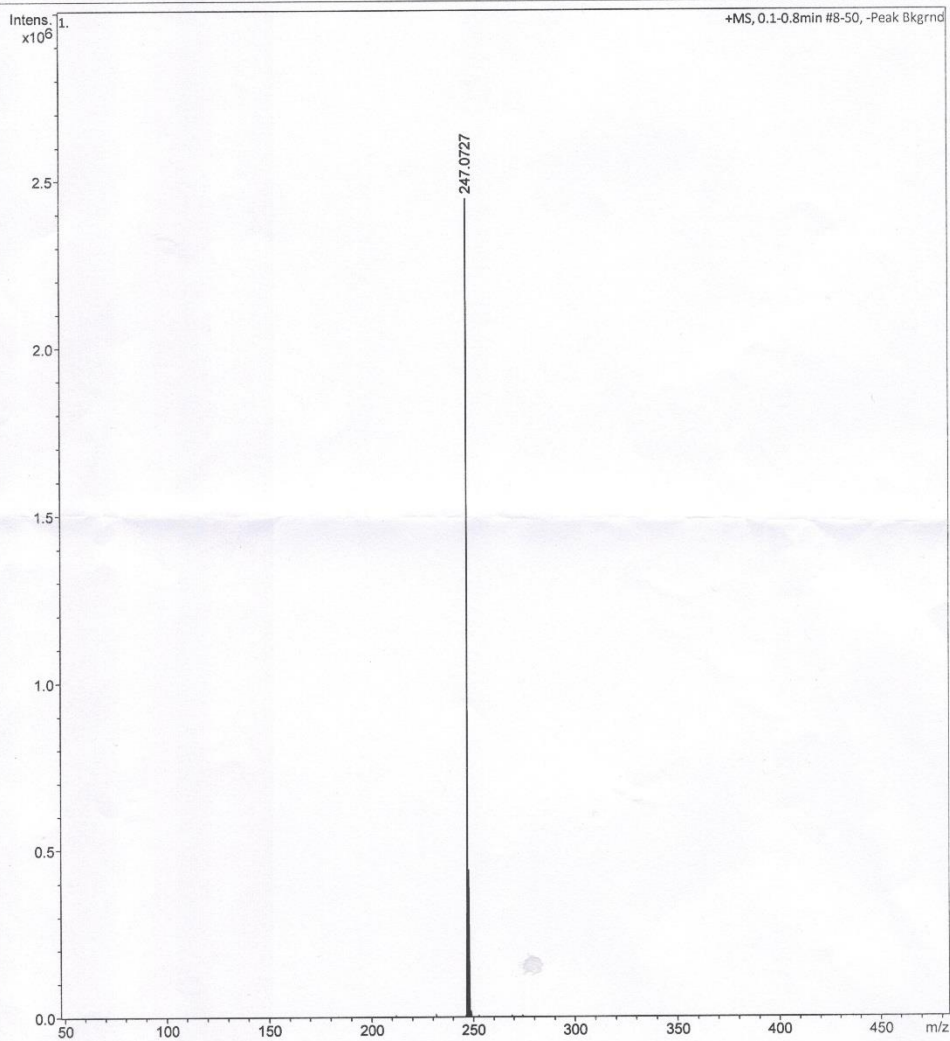
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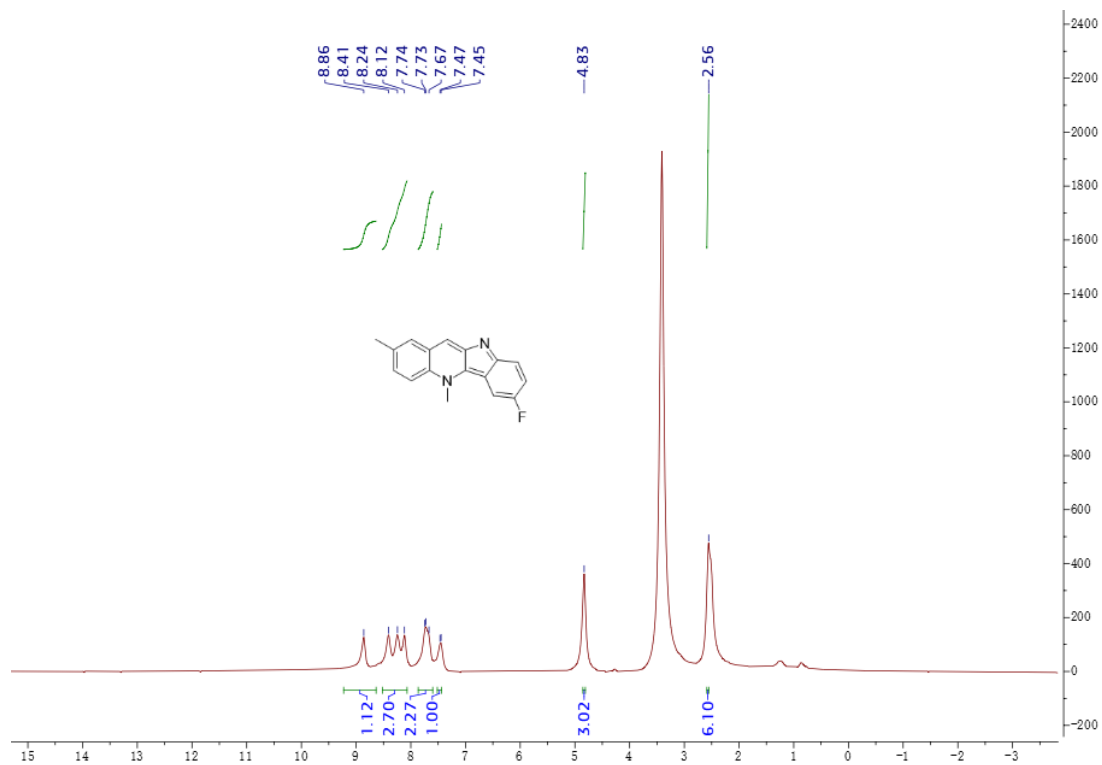
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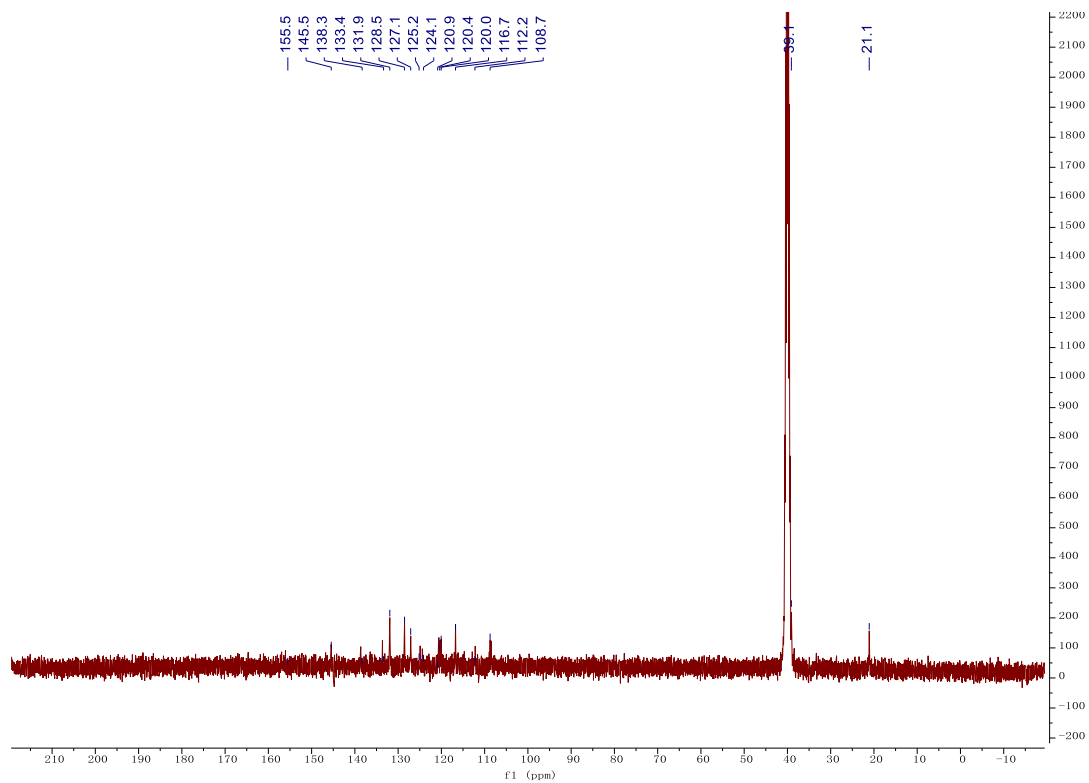
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The Mass spectrogram of compound **9**



The ^1H NMR spectrogram of compound **18**



The ^{13}C NMR spectrogram of compound **18**

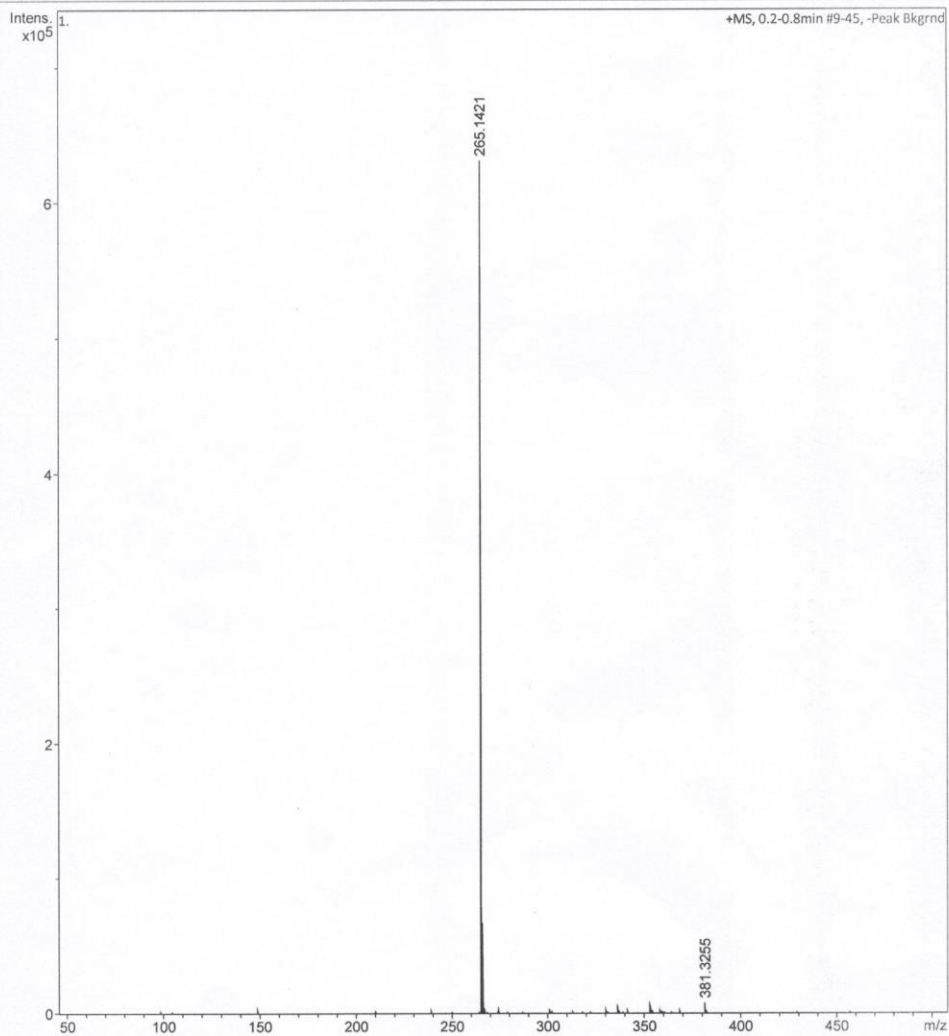
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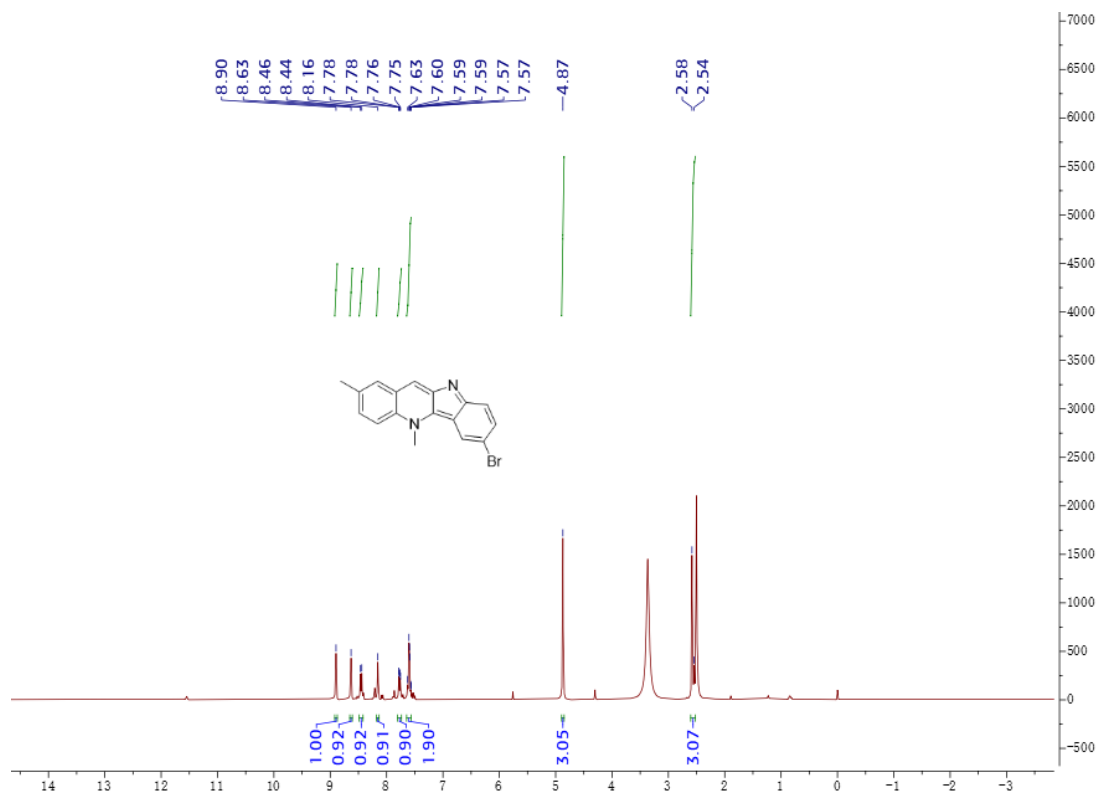
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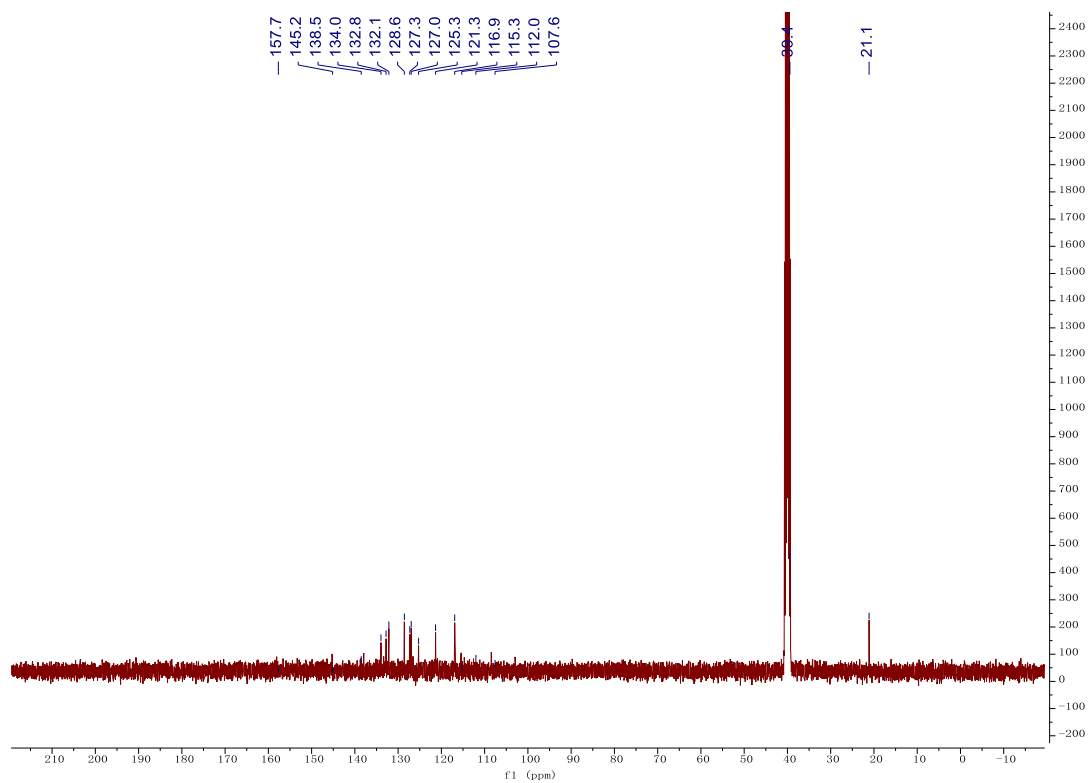
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The Mass spectrogram of compound **18**



The ^1H NMR spectrogram of compound 20



The ^{13}C NMR spectrogram of compound 20

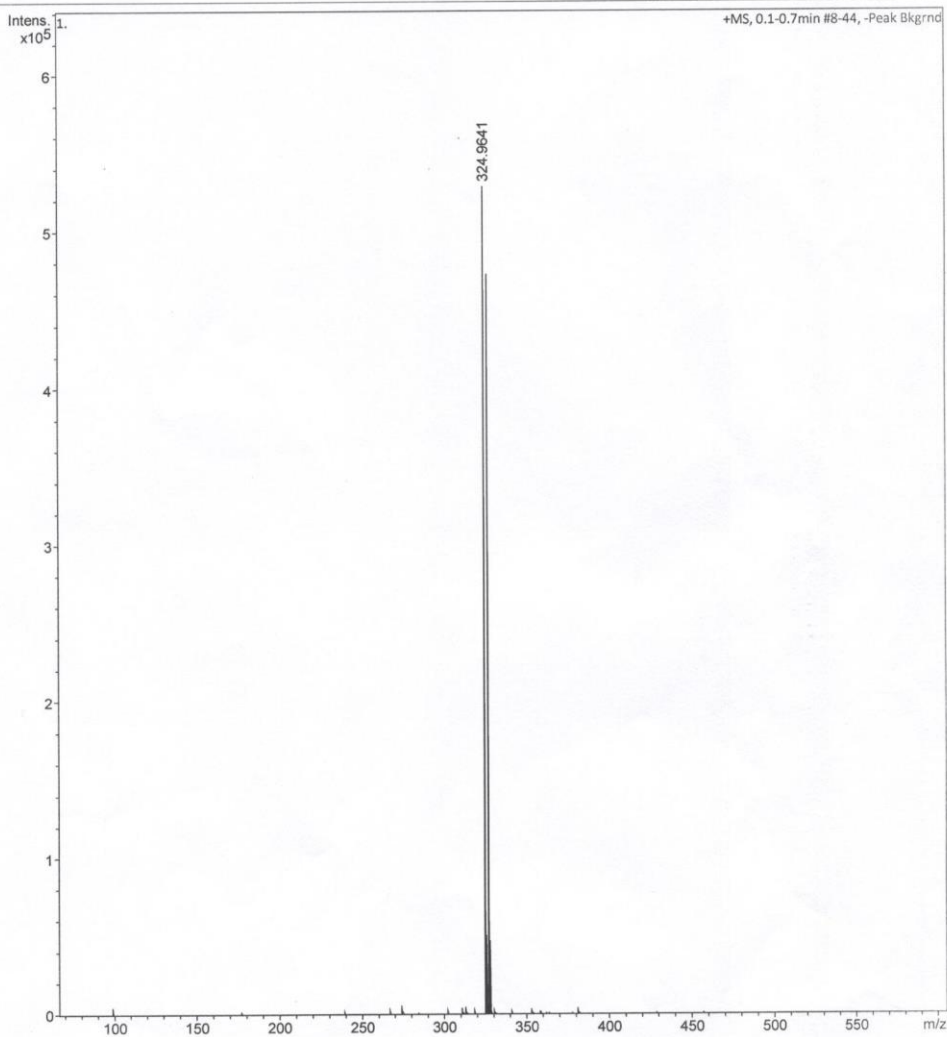
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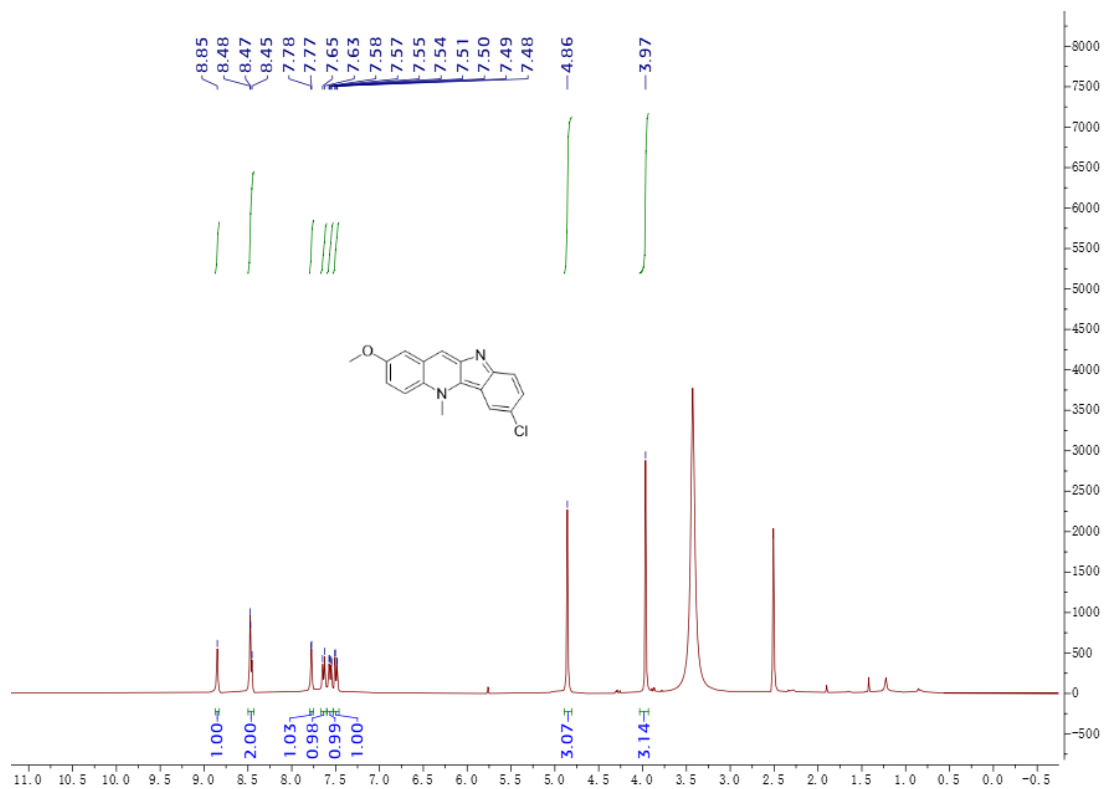
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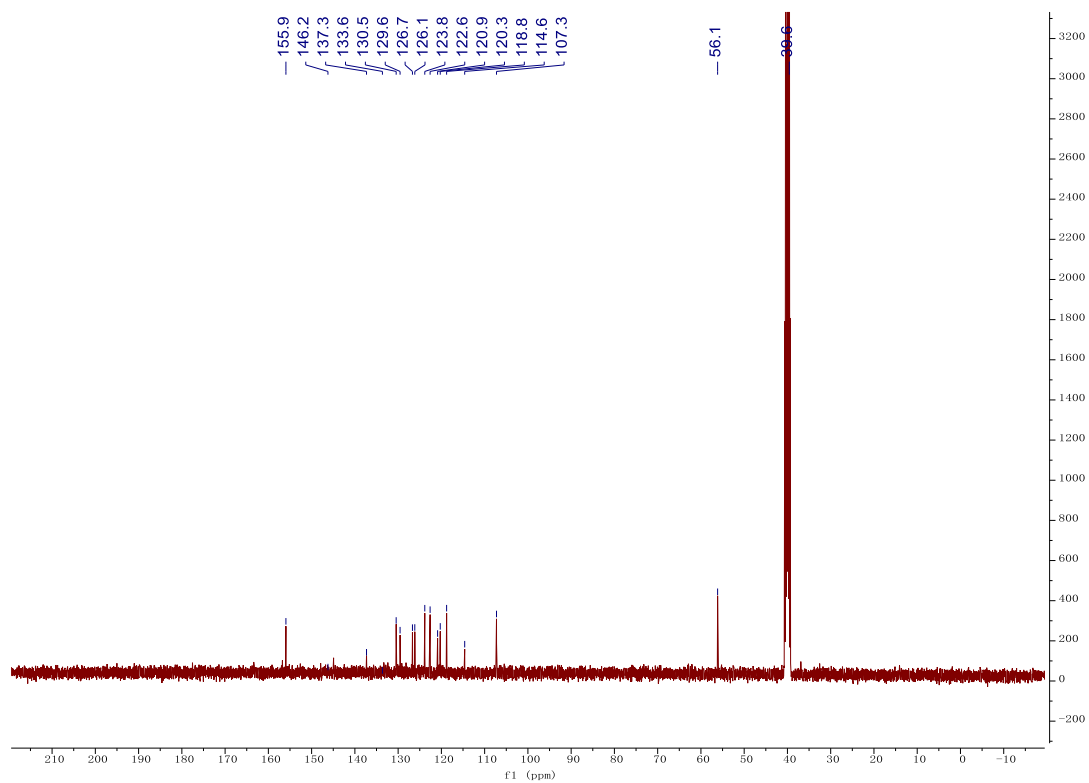
Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **20**



The ^1H NMR spectrogram of compound **21**



The ^{13}C NMR spectrogram of compound **21**

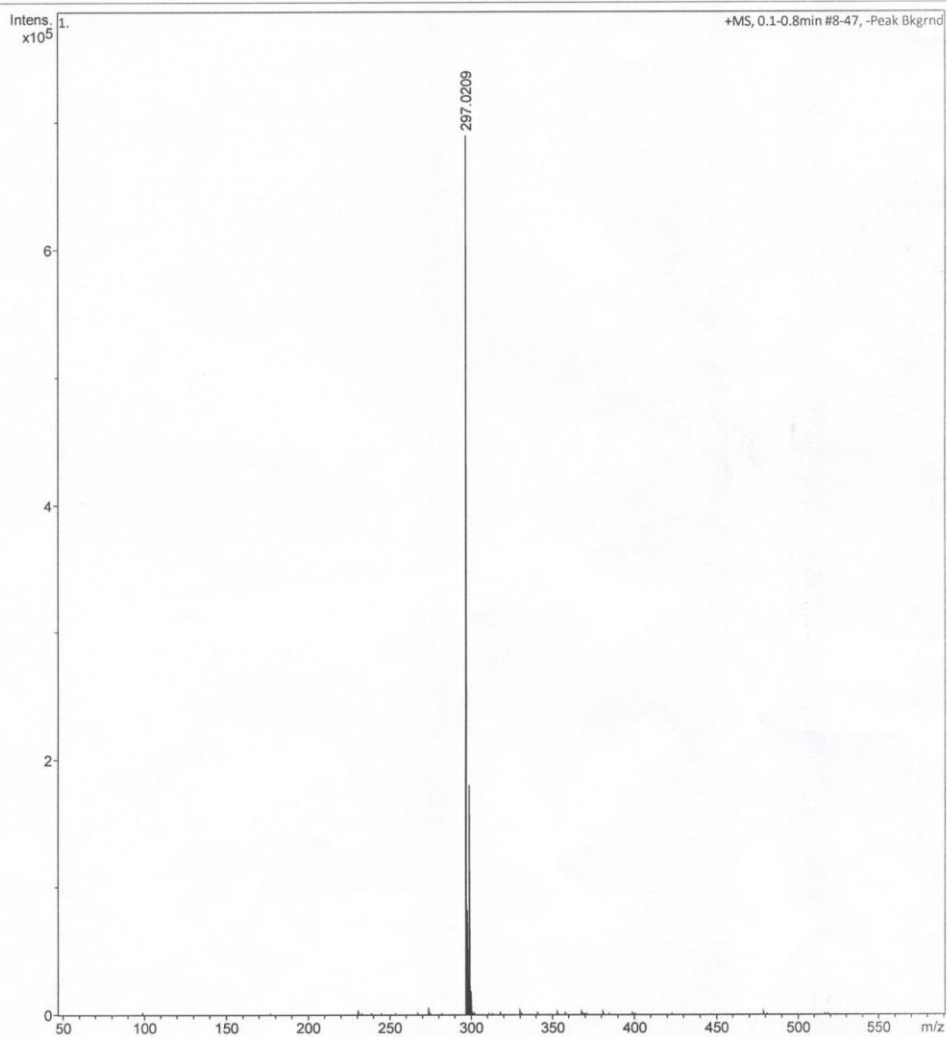
Generic Display Report

Analysis Info

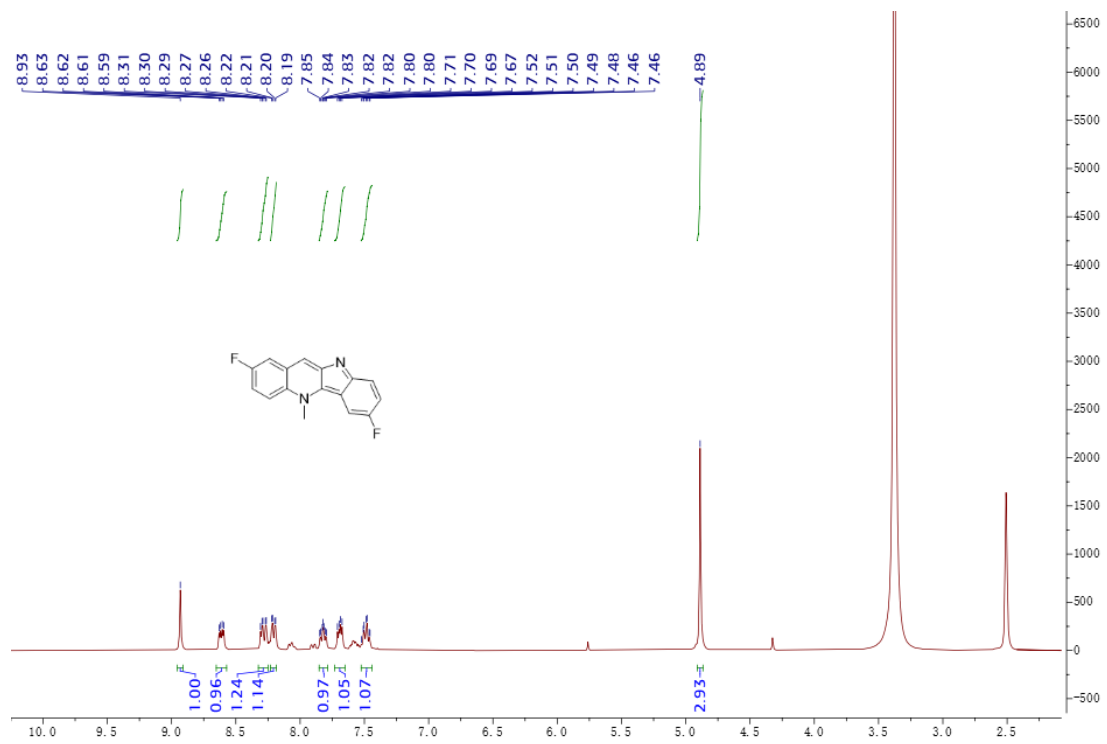
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Comment

Acquisition Date 10/29/2020 12:55:14 PM

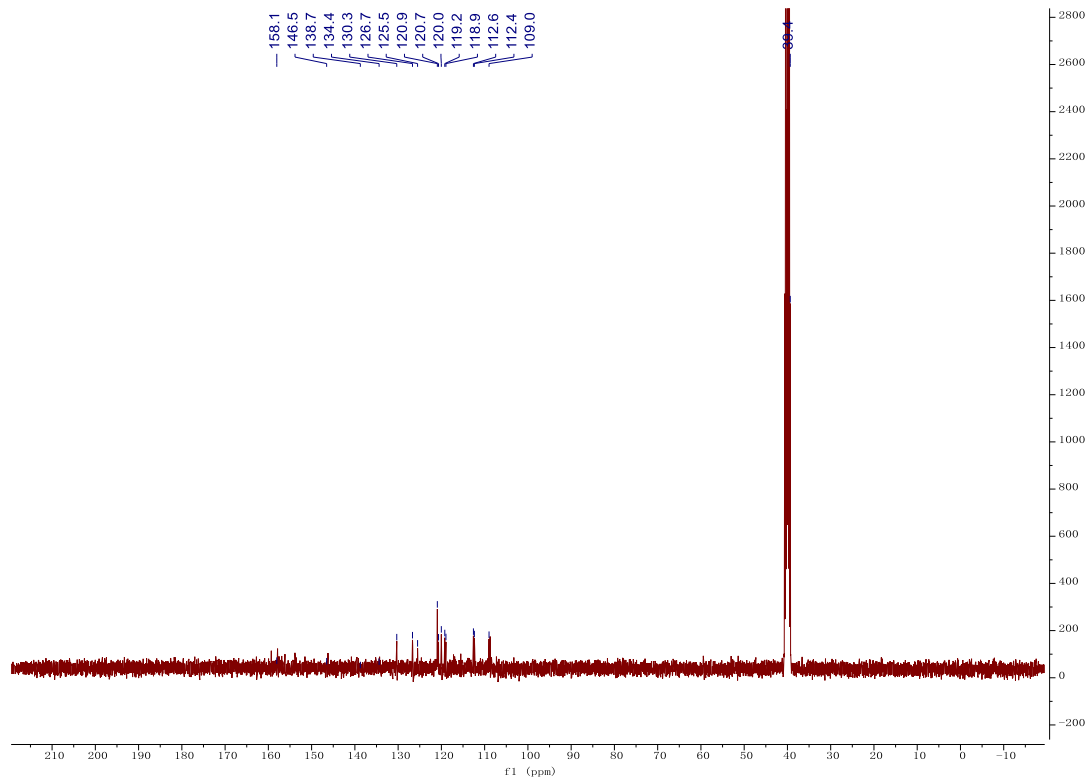
Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **21**



The ^1H NMR spectrogram of compound 22



The ^{13}C NMR spectrogram of compound 22

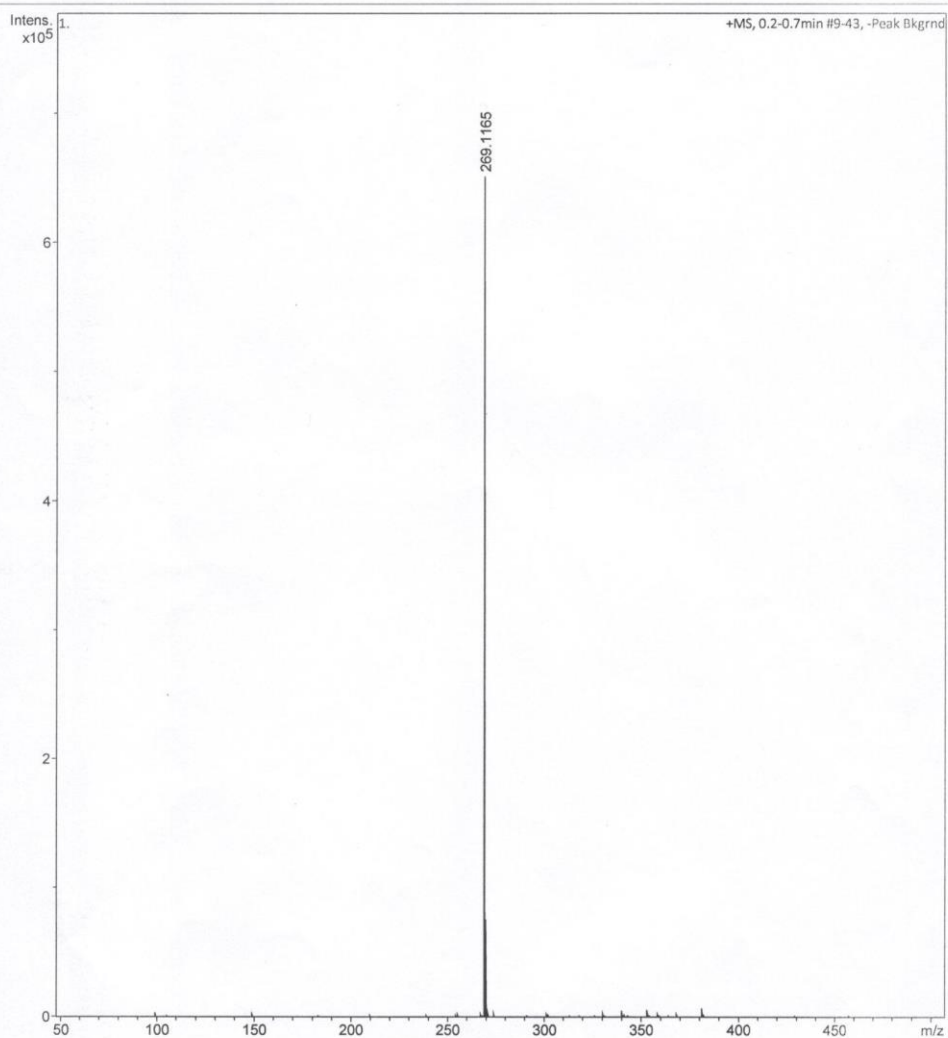
Generic Display Report

Analysis Info

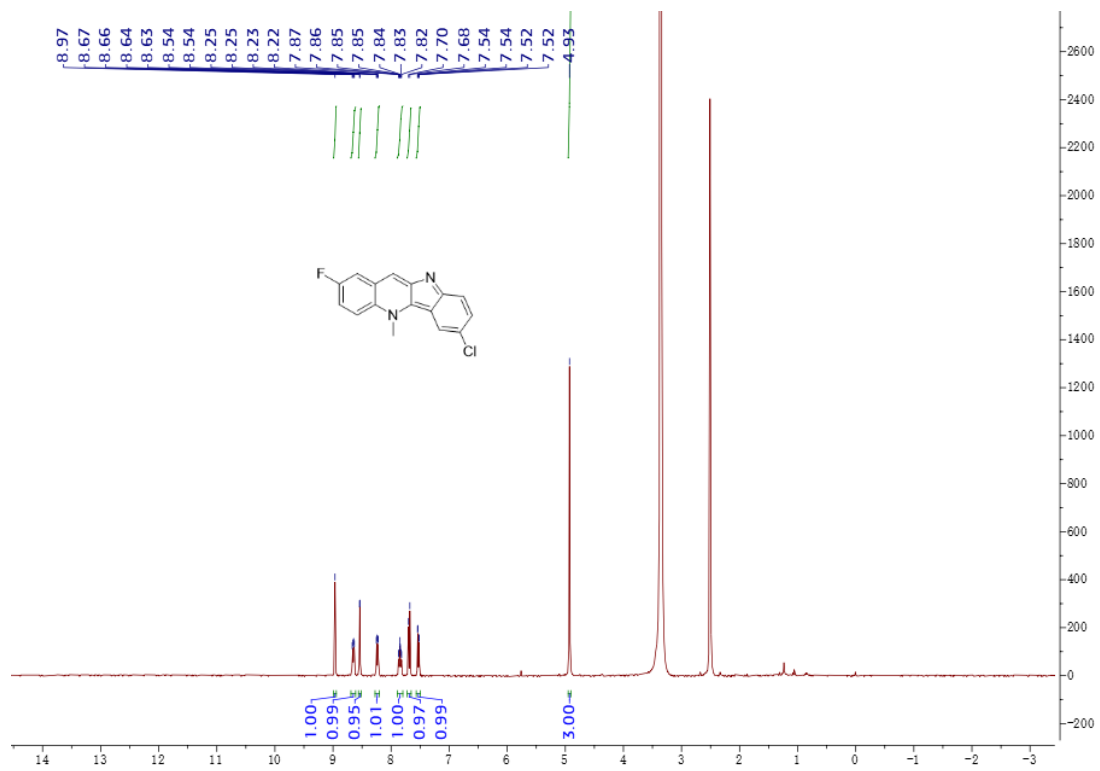
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Acquisition Date 12/16/2020 12:27:44 PM

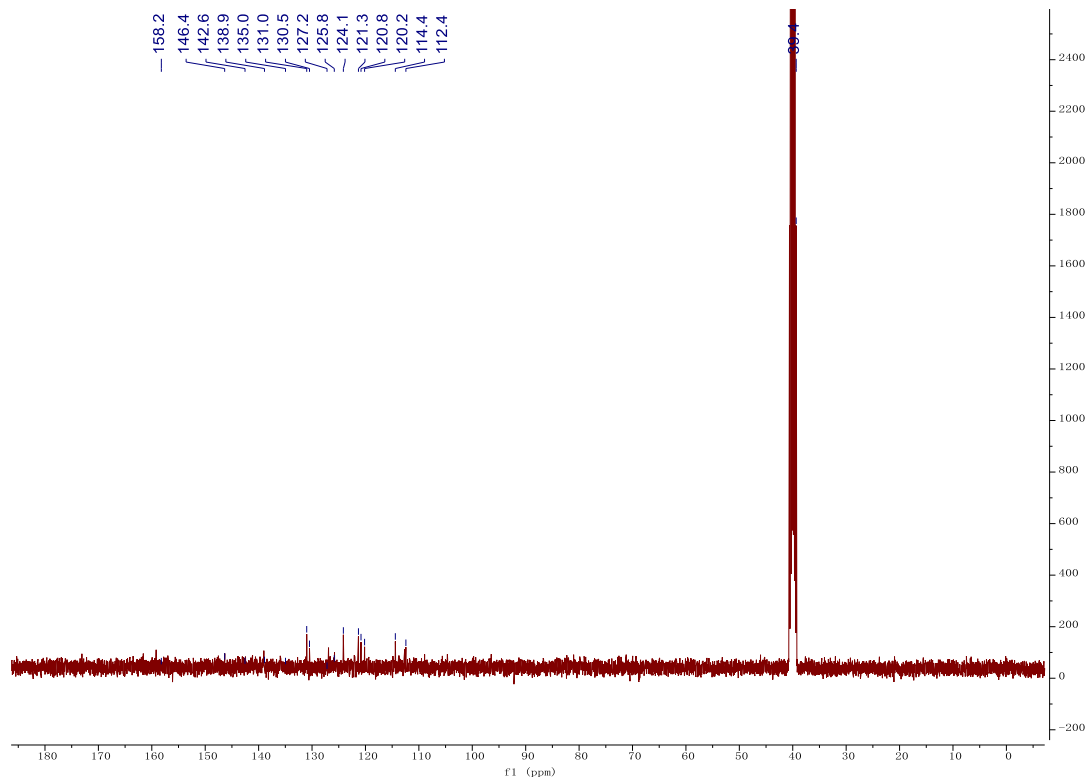
Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **22**



The ^1H NMR spectrogram of compound **23**



The ^{13}C NMR spectrogram of compound **23**

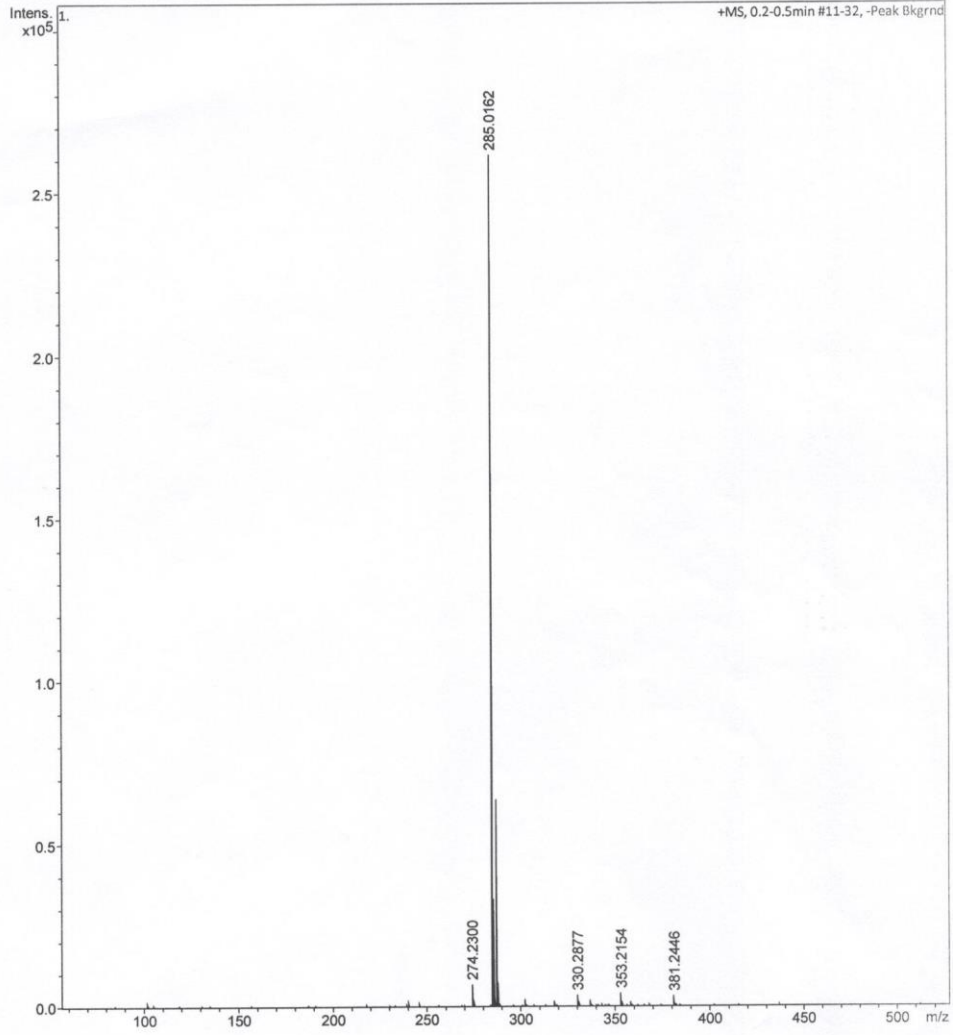
Generic Display Report

Analysis Info

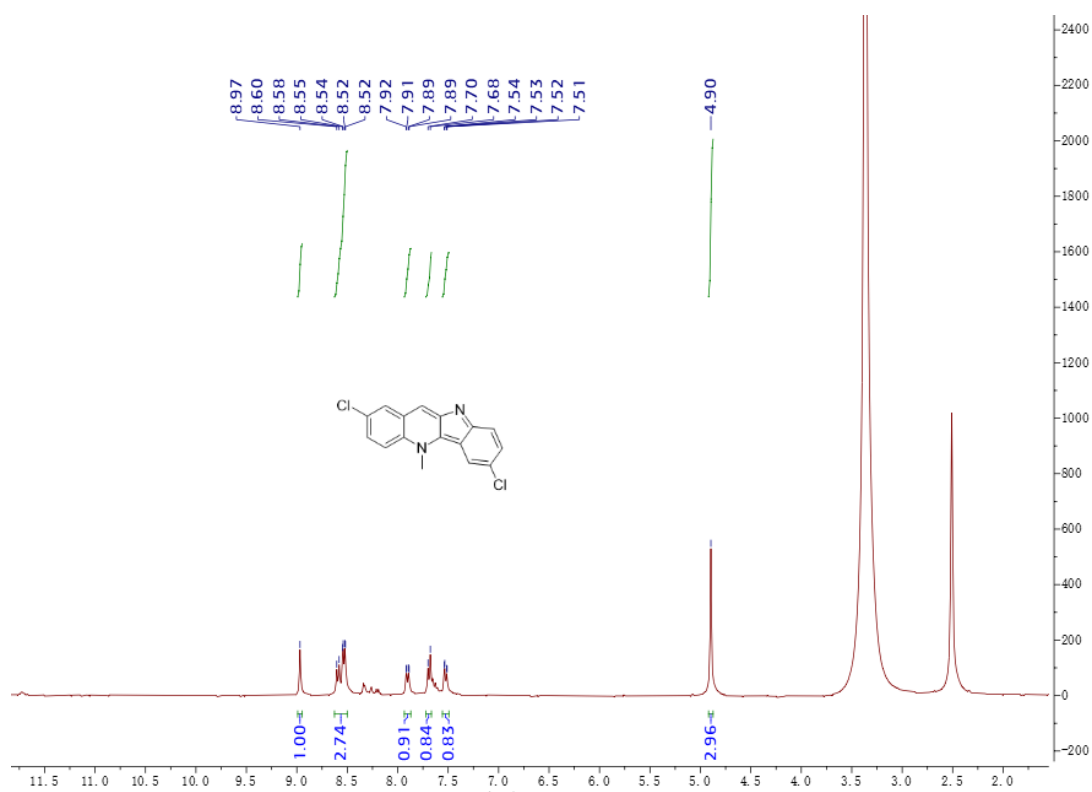
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Acquisition Date 11/17/2020 1:15:59 PM

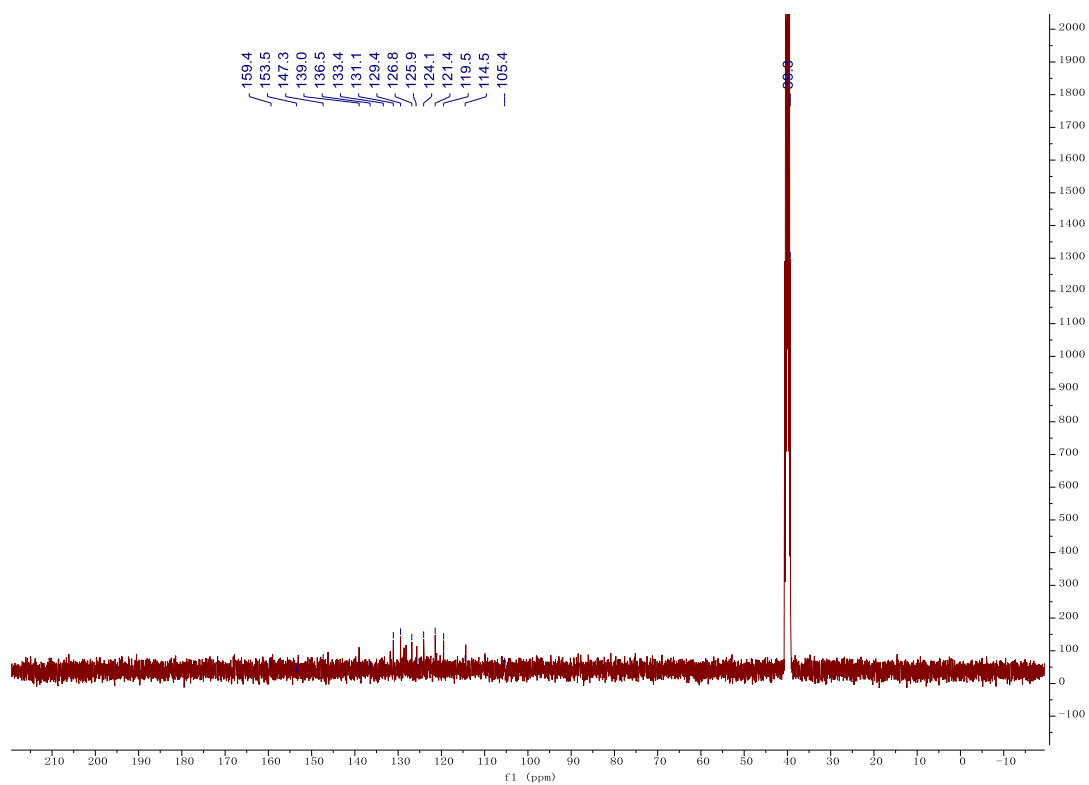
Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **23**



The ^1H NMR spectrogram of compound **25**



The ^{13}C NMR spectrogram of compound **25**

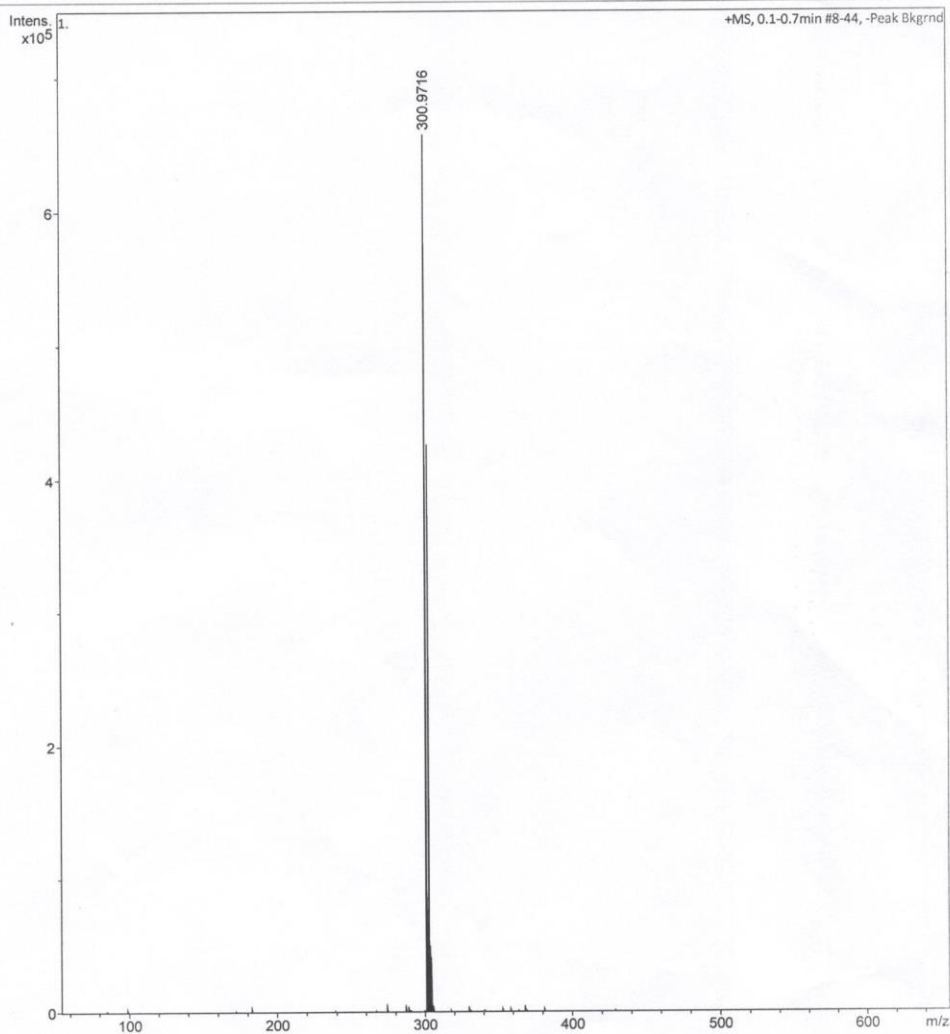
Generic Display Report

Analysis Info

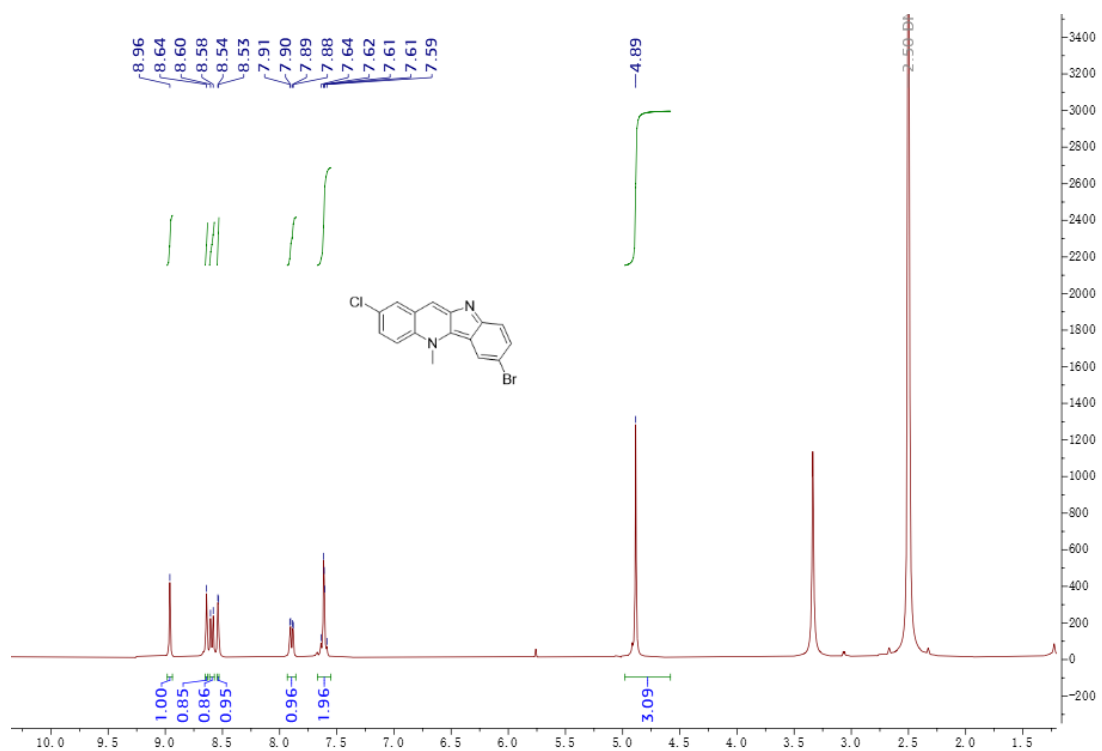
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Acquisition Date 11/2/2020 1:20:09 PM

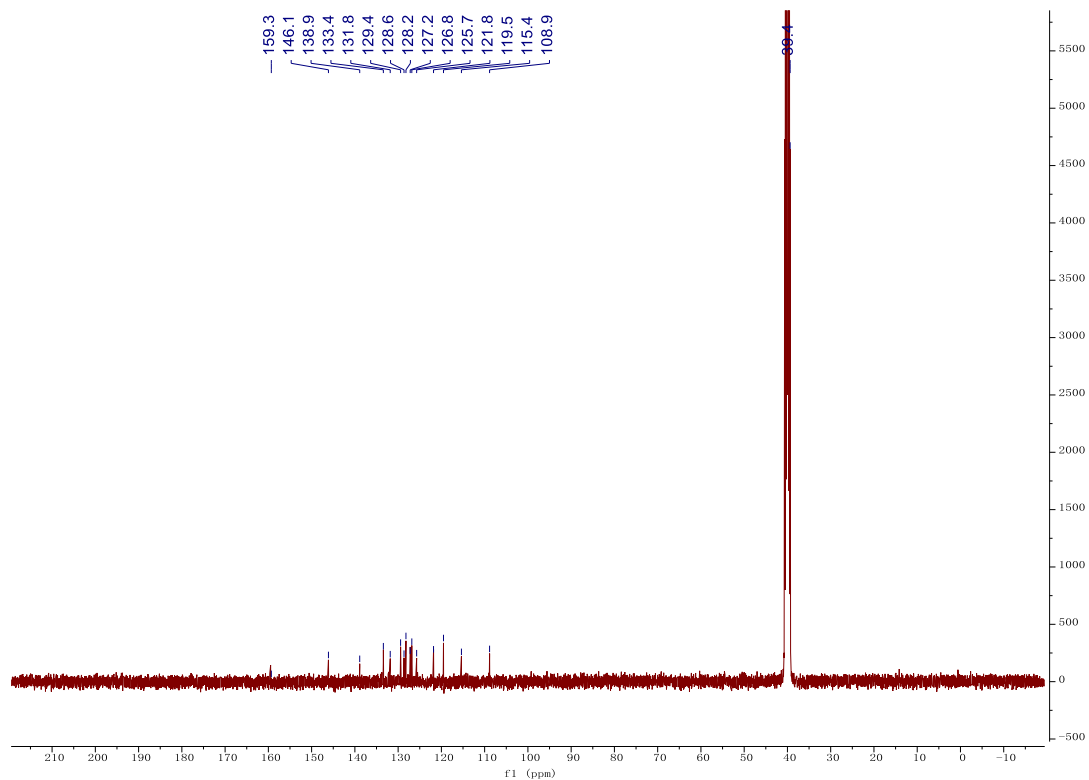
Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **25**



The ^1H NMR spectrogram of compound 26



The ^{13}C NMR spectrogram of compound 26

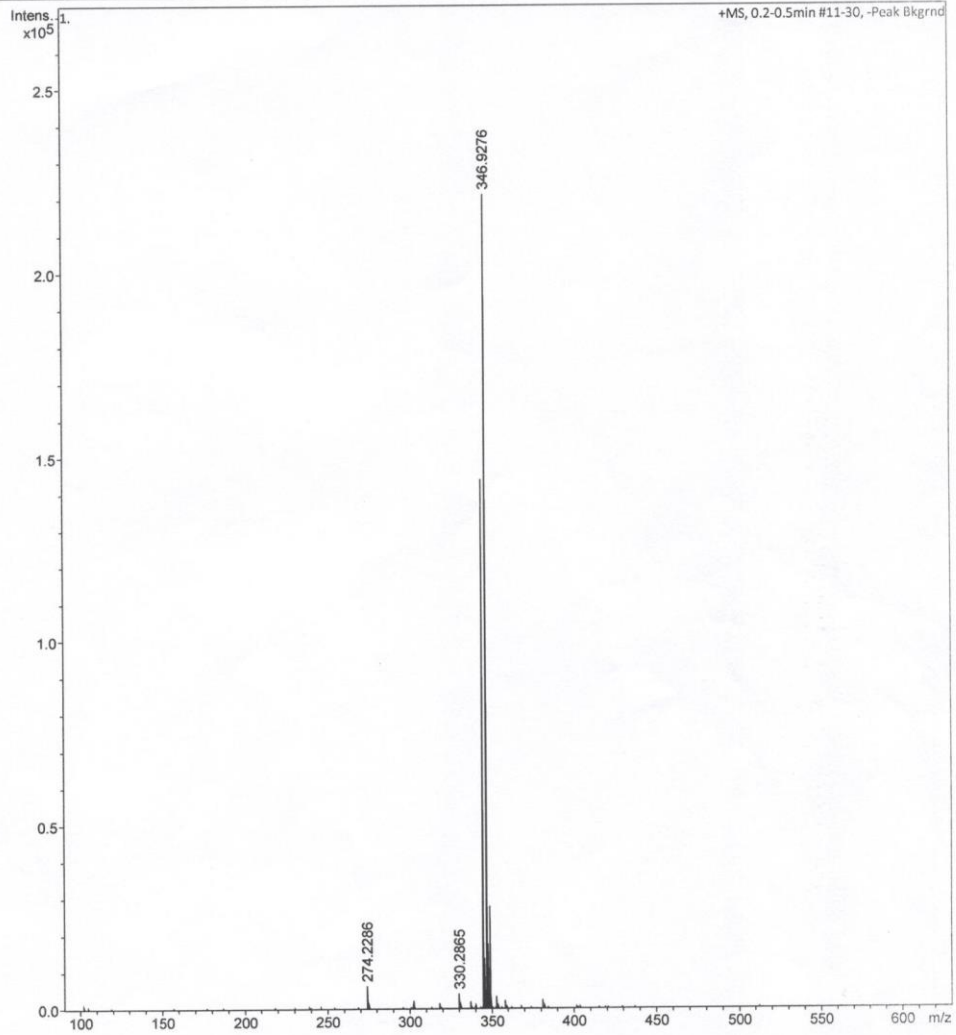
Generic Display Report

Analysis Info

Analysis Name D:\Data\yangy\new\CHUQINGRU201117_1_28_01_35354.d
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Sample Name CHUQINGRU201117_1
Comment

Acquisition Date 11/17/2020 1:12:57 PM

Operator LZU
Instrument micrOTOF



The Mass spectrogram of compound **26**

4. In Vivo Antibacterial Activity.

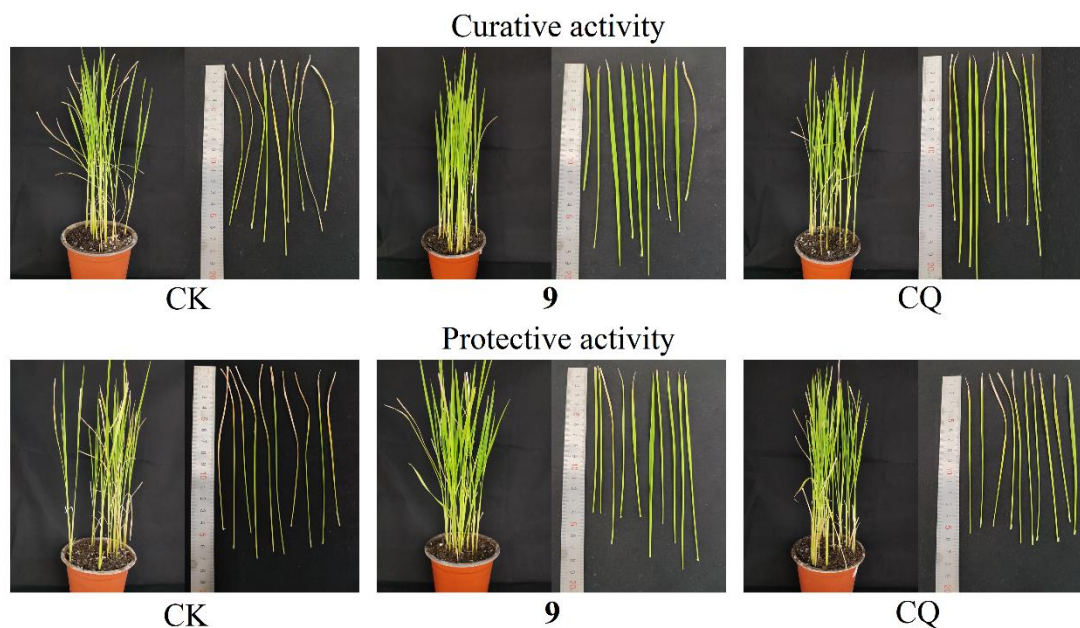


Figure S1. Curative and protective activities of compound **9** against rice bacterial leaf blight at 200 mg/L. CK, negative control; CQ, copper quinolate.

5. Molecular docking in detail.

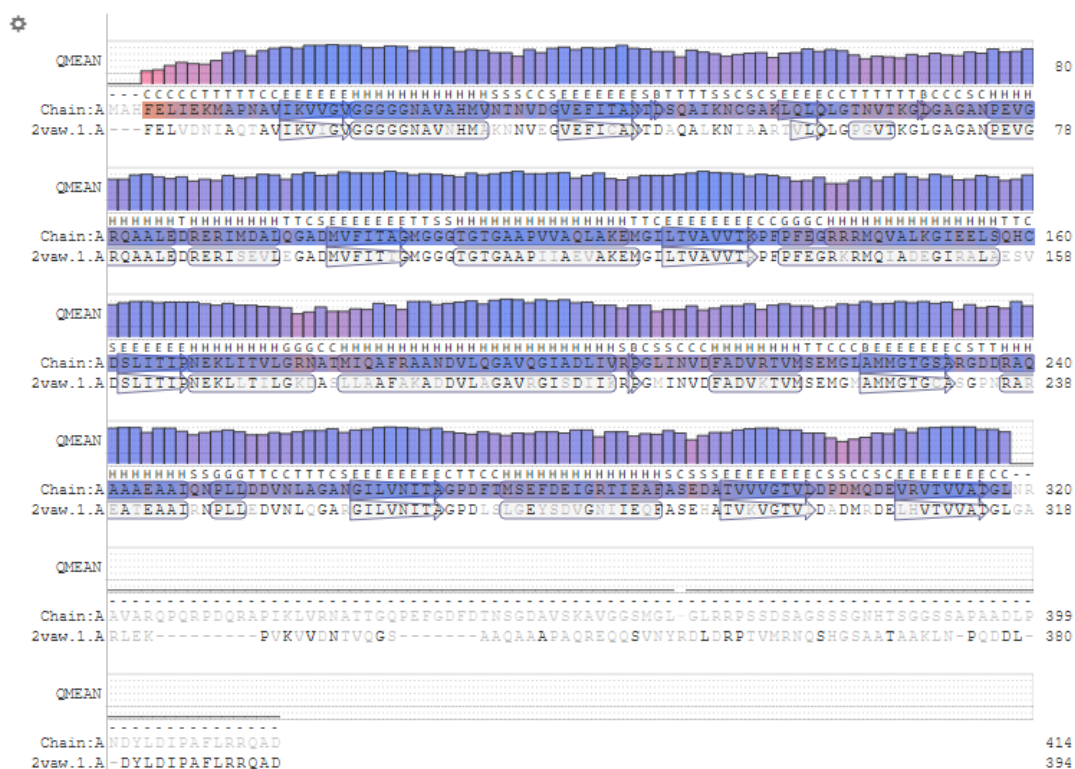


Figure S2. Sequence alignment of *X. oryzae* *ftsZ* with the template.

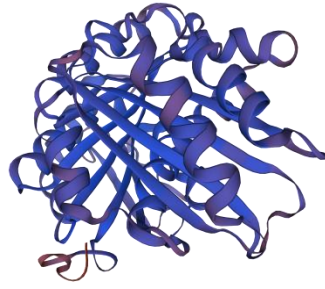


Figure S3. The crystal model of *X. oryzae ftsZ* protein.

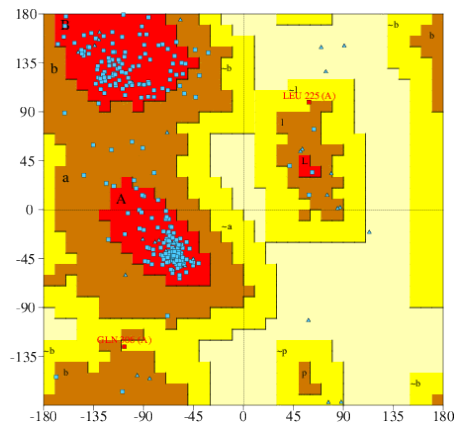


Figure S4. Ramachandran plot of the *X. oryzae ftsZ* protein model.

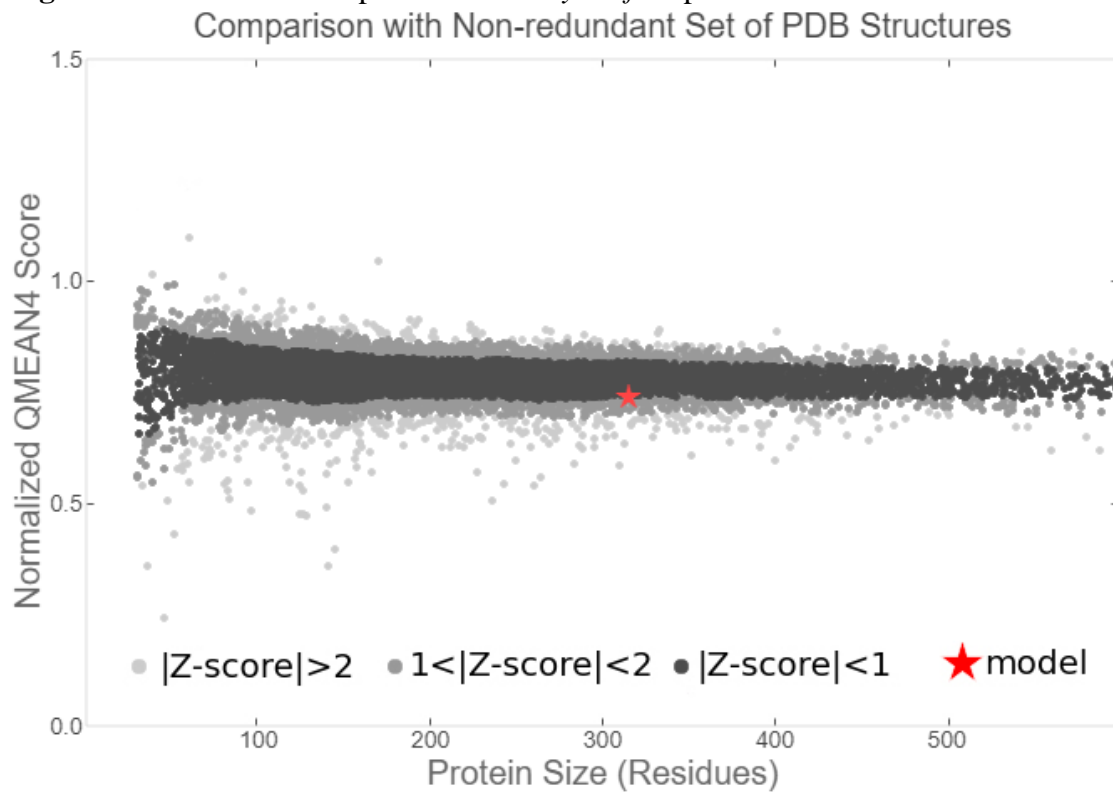


Figure S5. Z-plot of *ftsZ* protein.

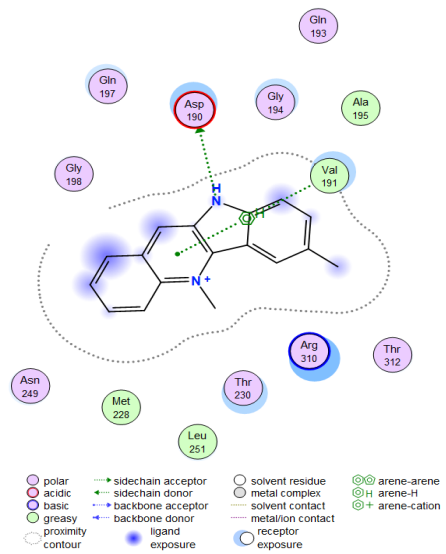
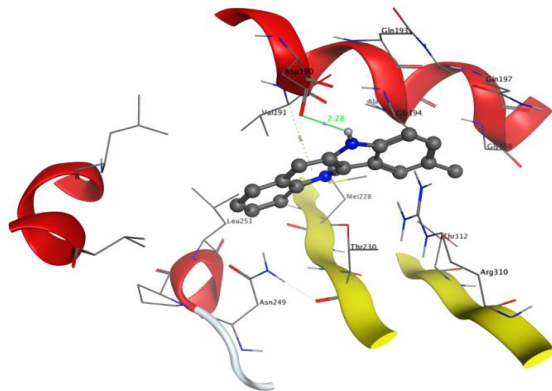


Figure S6. Docking results.