

Supplementary Materials

Dess–Martin Periodinane-Mediated Oxidative Coupling Reaction of Isoquinoline with Benzyl Bromide

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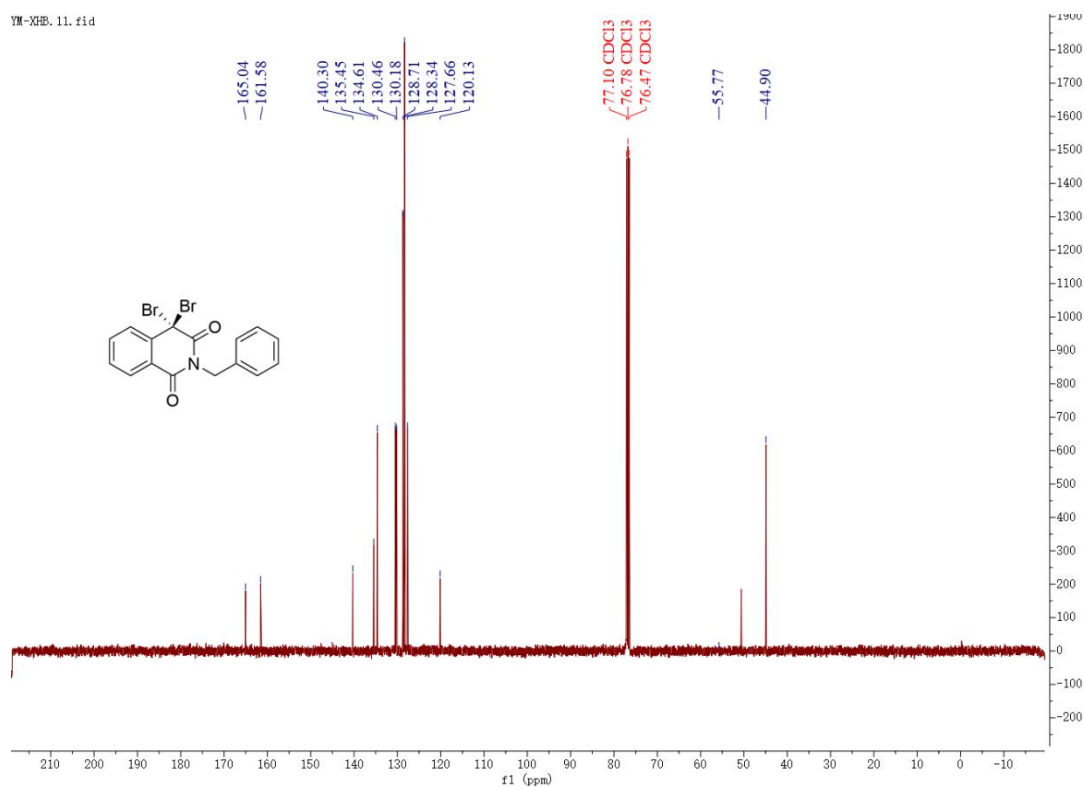
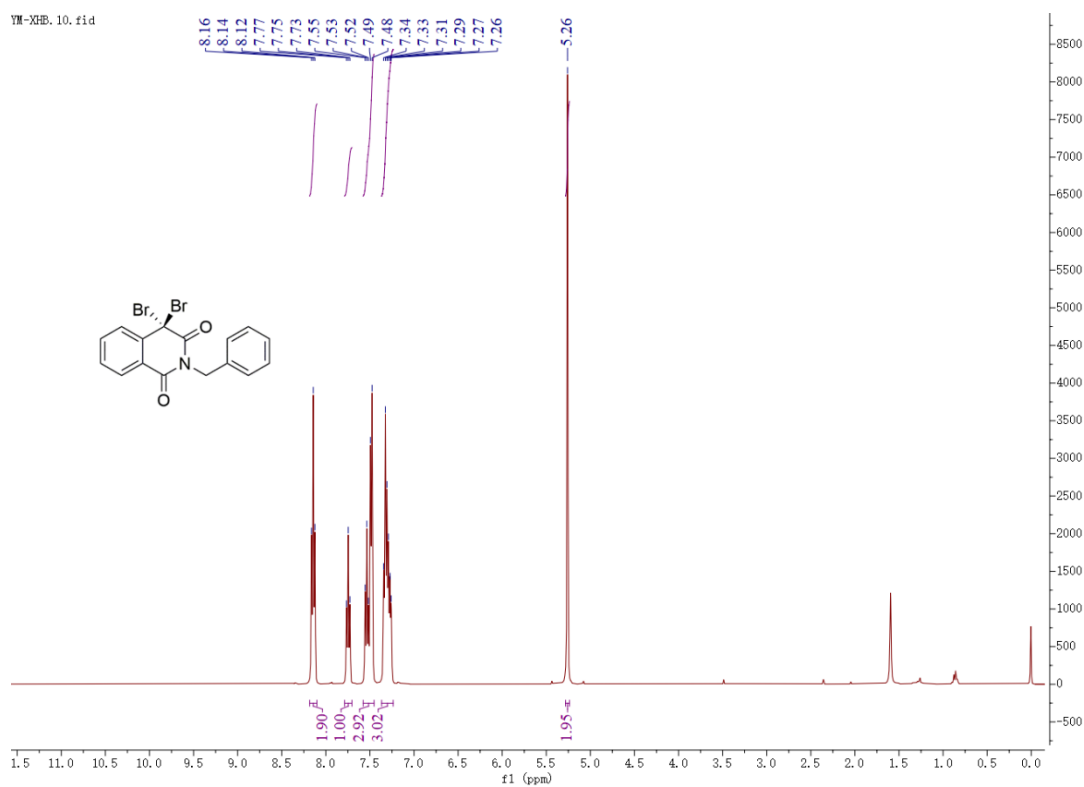
¹ Natural Products Research Centre, Chengdu Institute of Biology, Chinese Academy of Sciences, Chengdu 610041, China

² University of Chinese Academy of Sciences, Beijing 100049, China

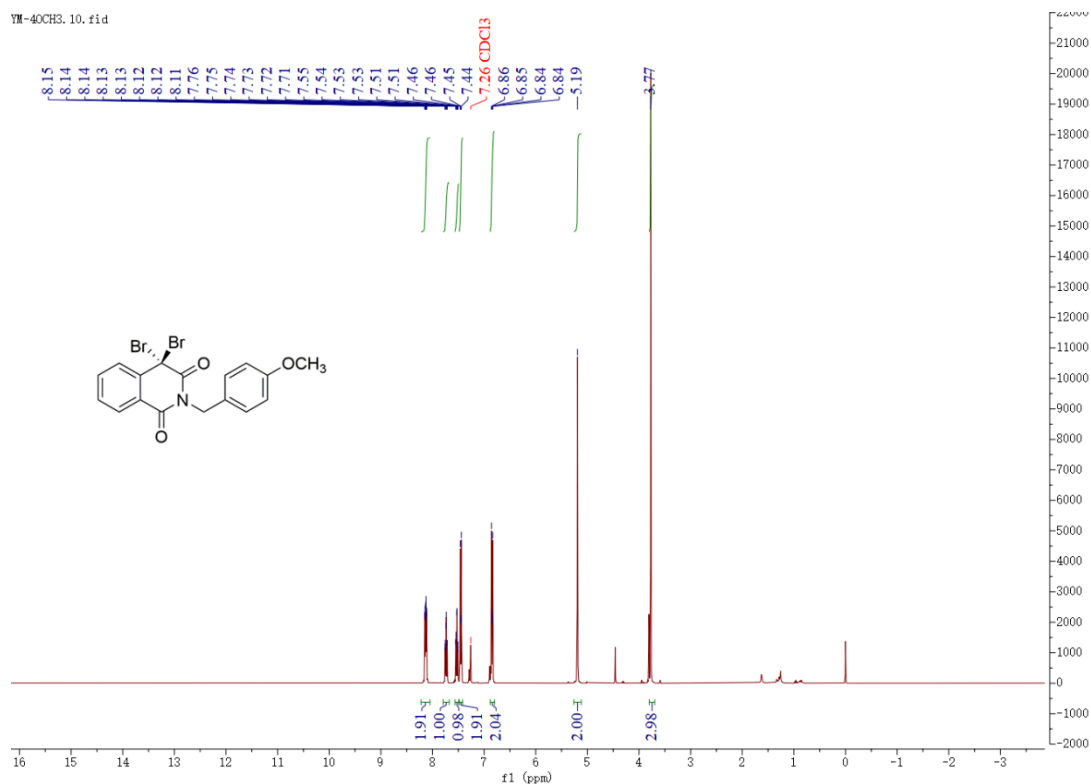
* Correspondence: jiaowei@cib.ac.cn

† These authors contributed equally to this work.

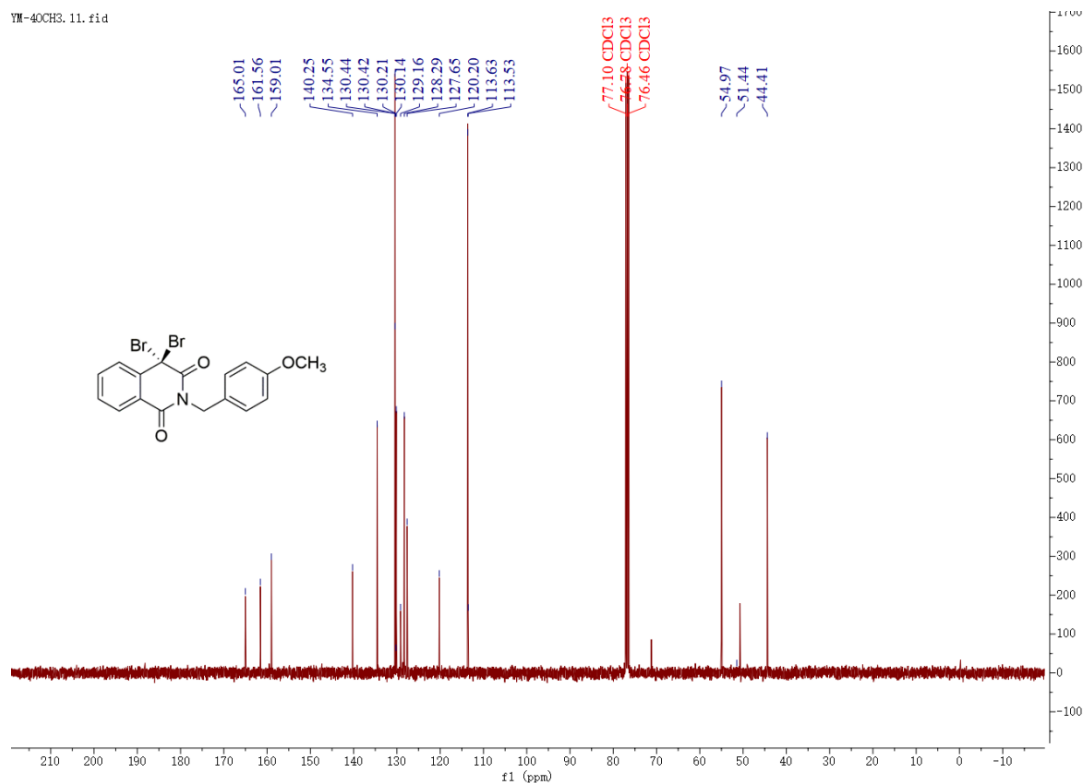
1. ^1H NMR and ^{13}C NMR spectra of the synthesized compounds



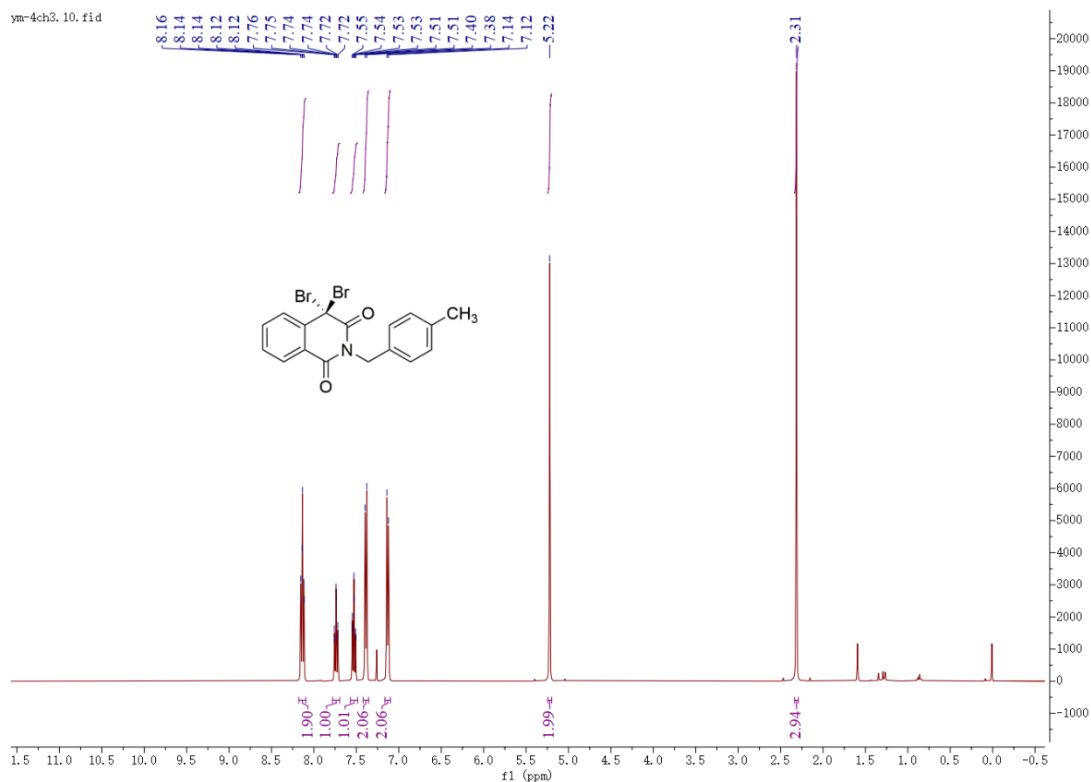
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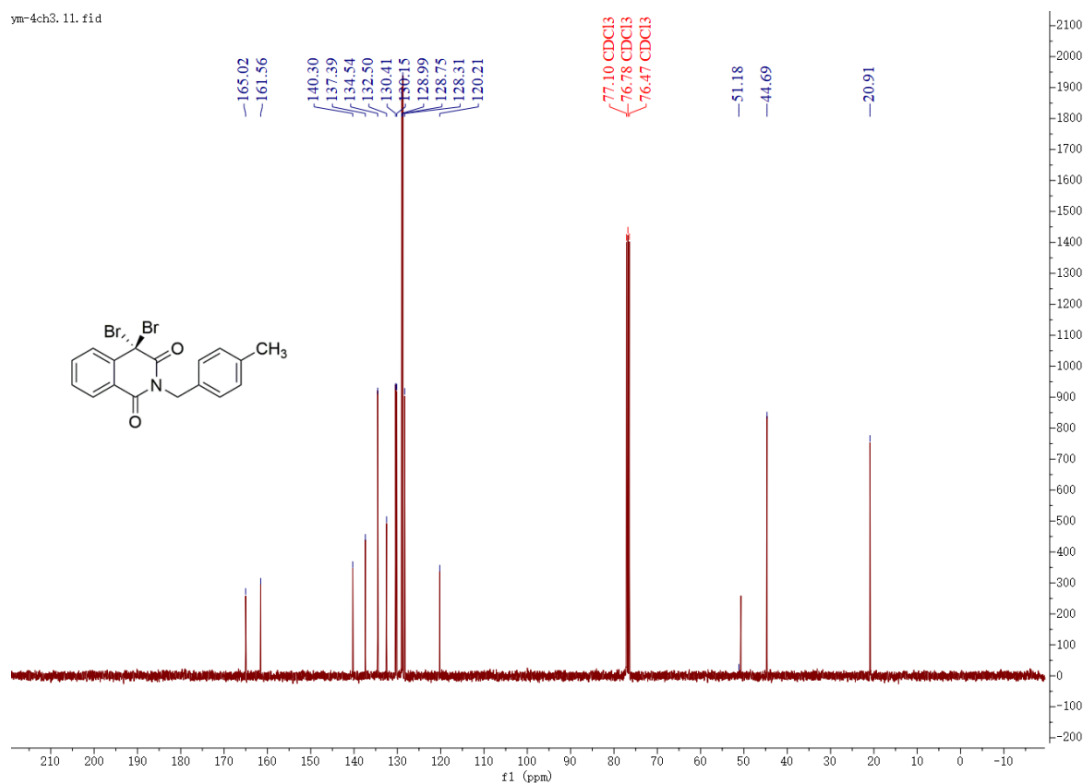
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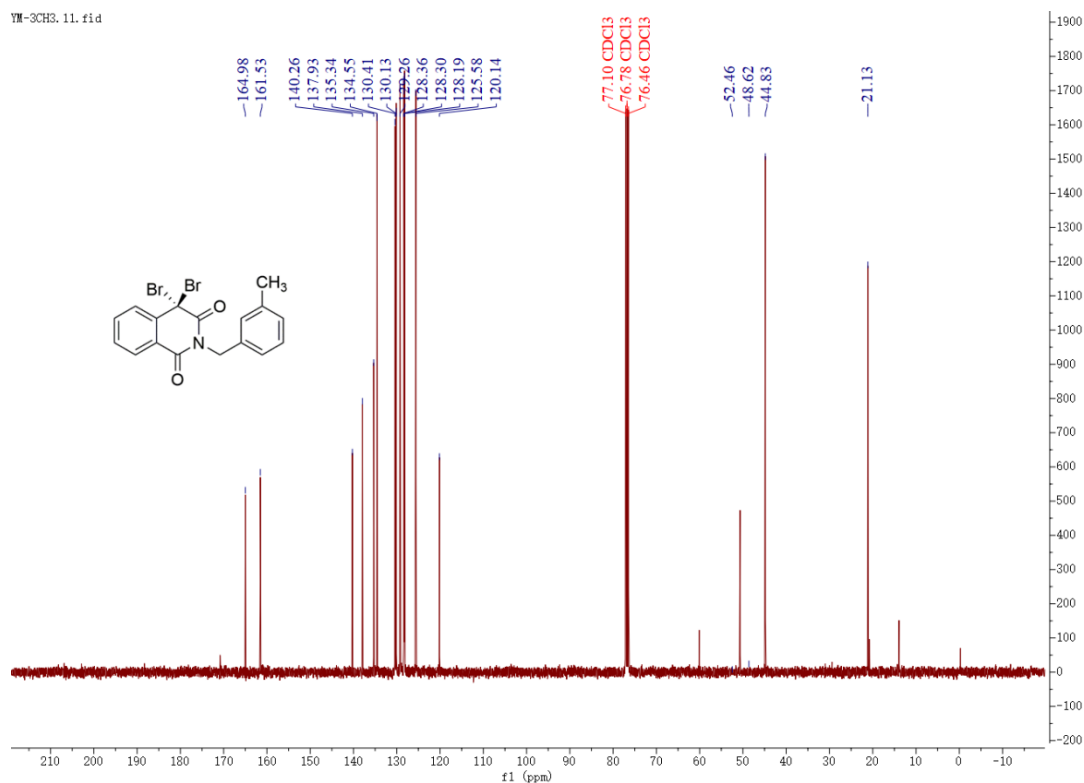
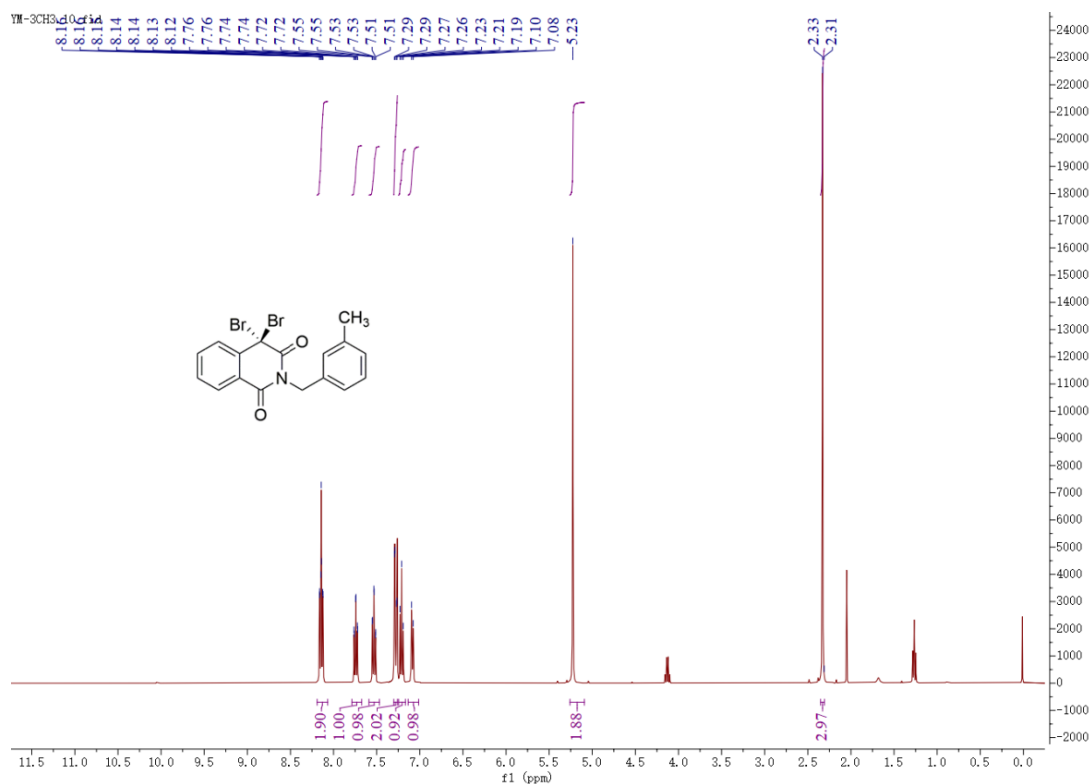


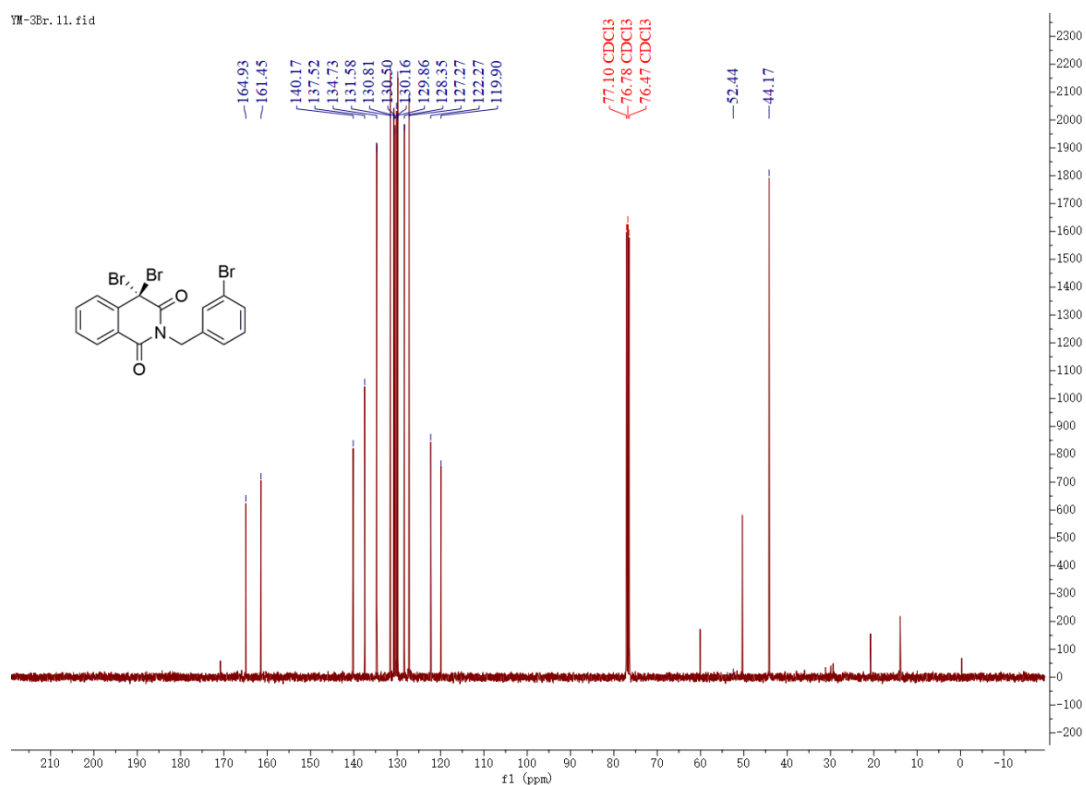
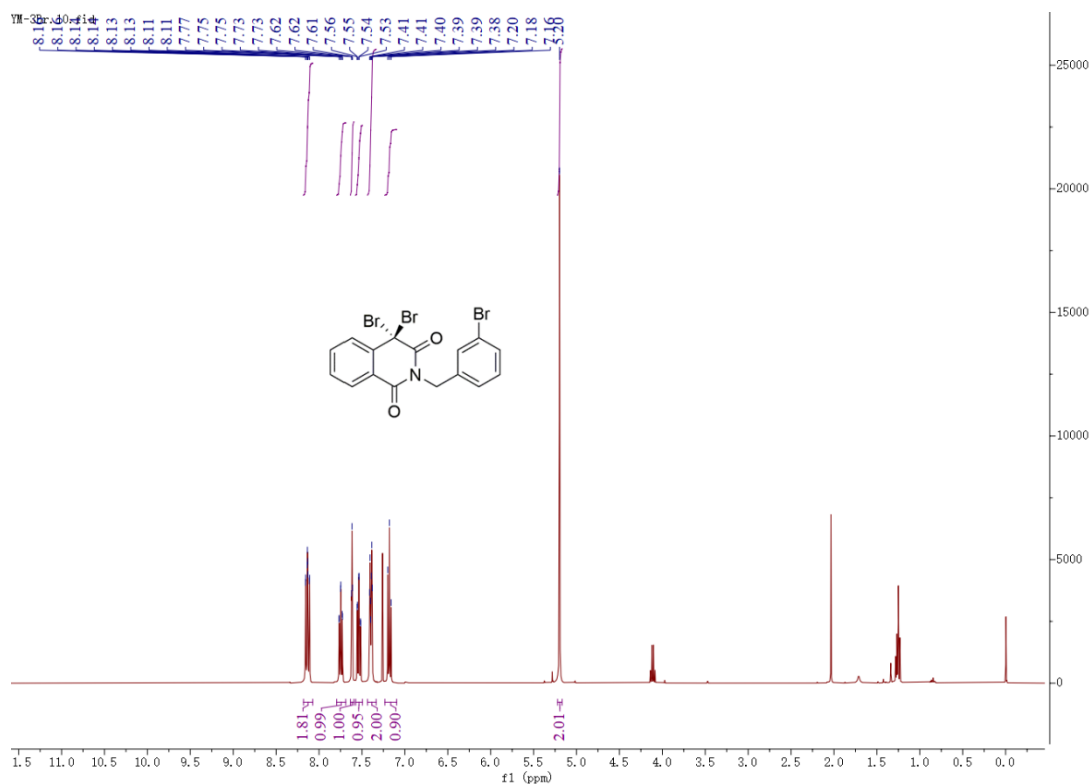
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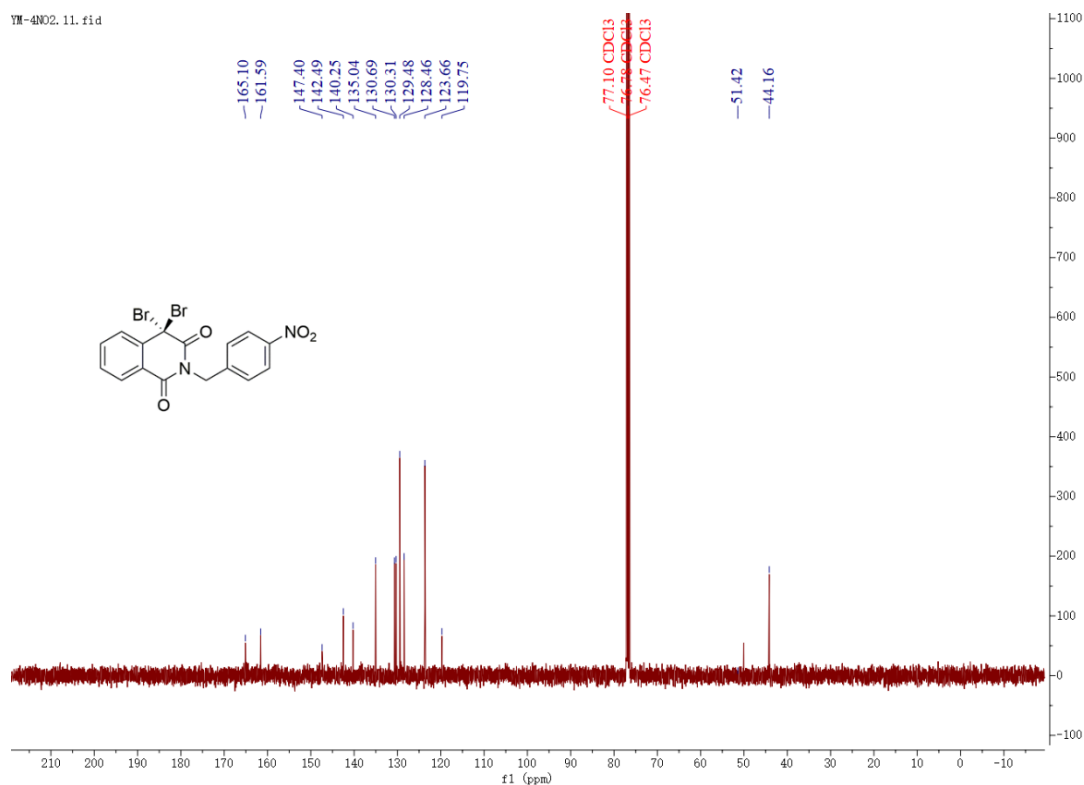
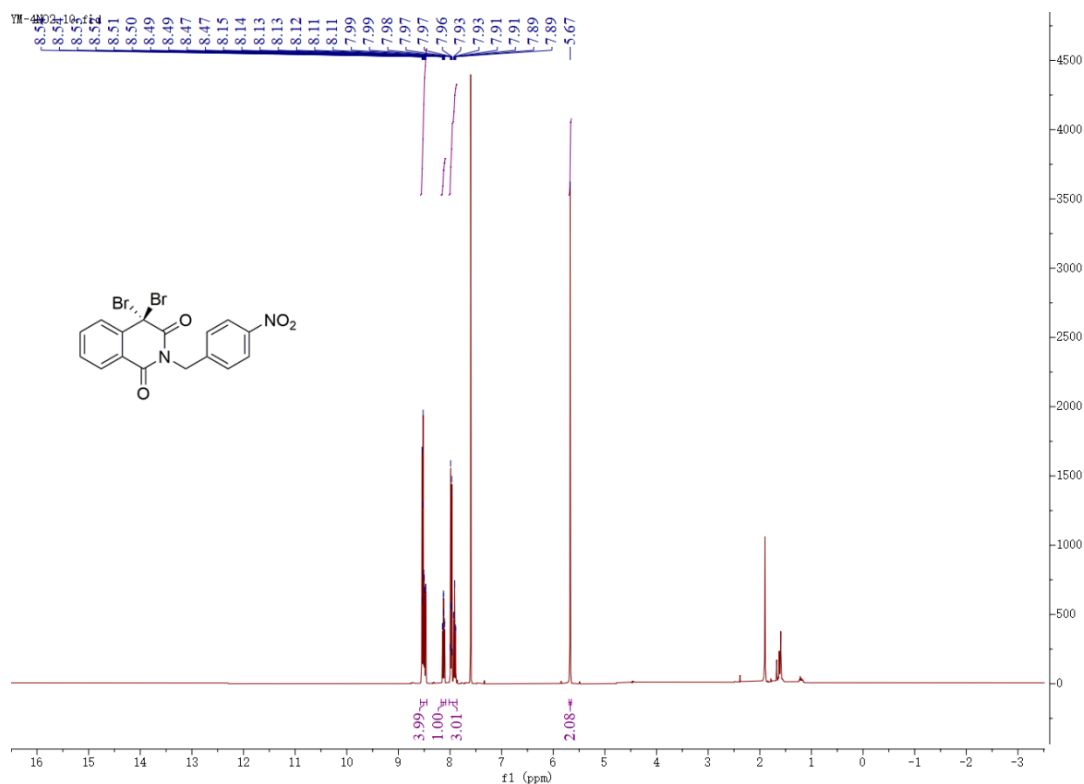


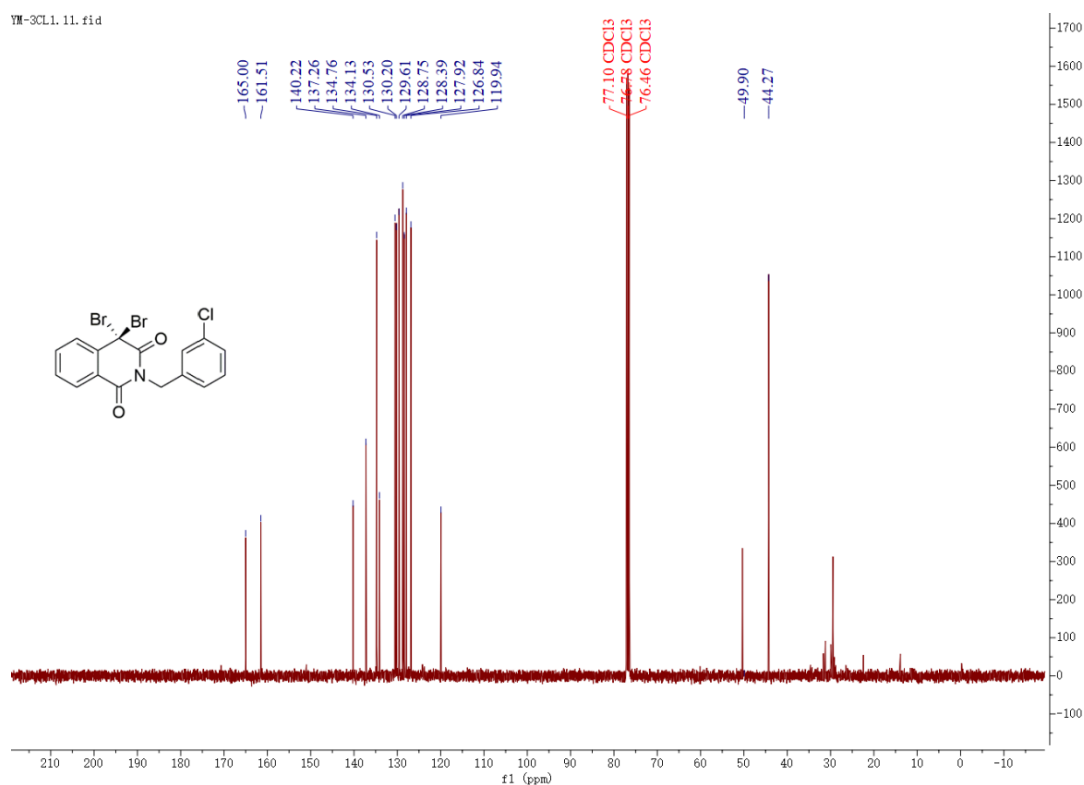
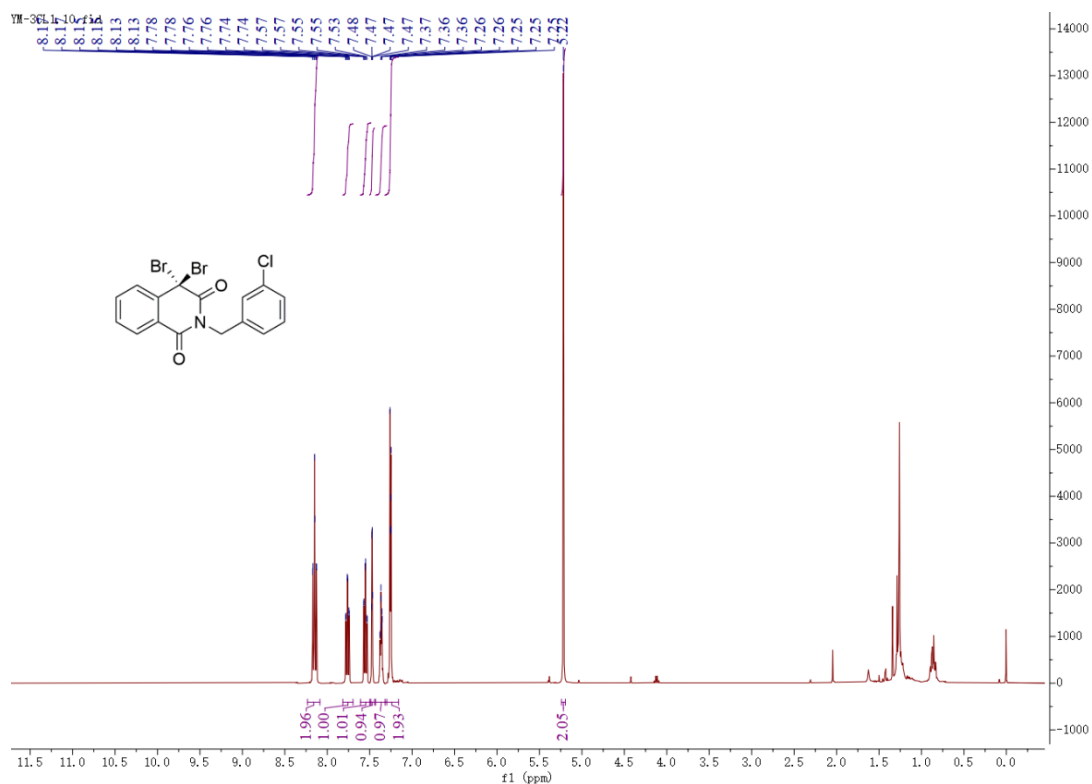
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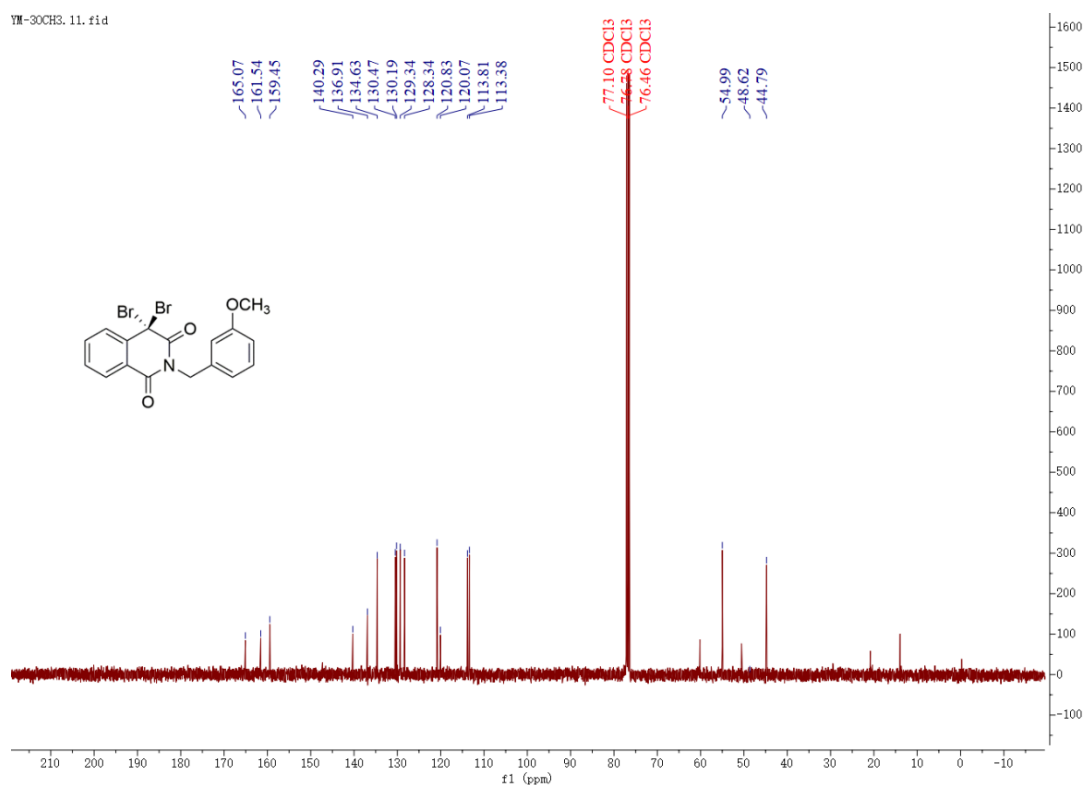
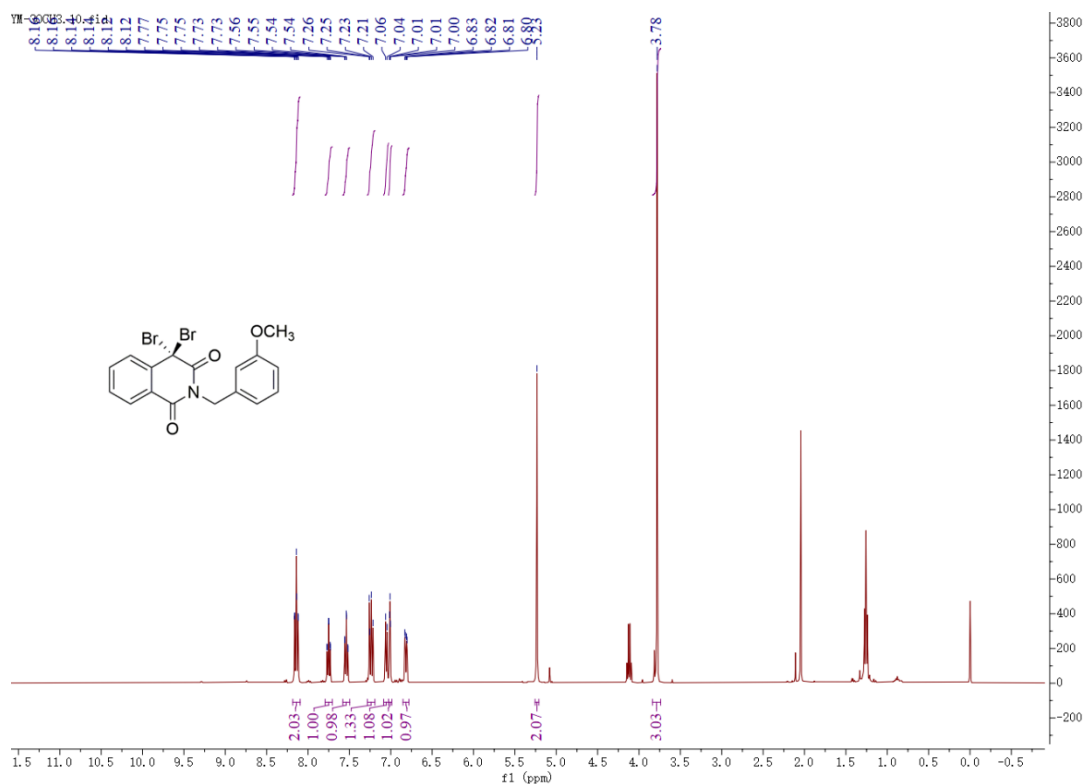


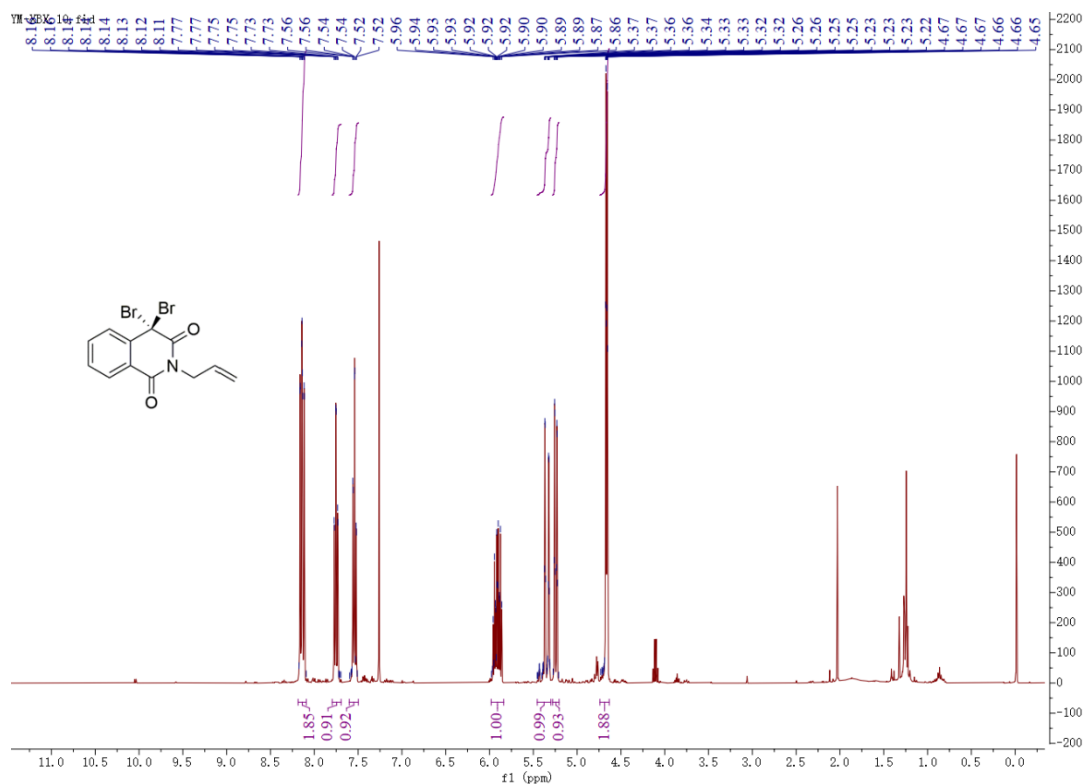




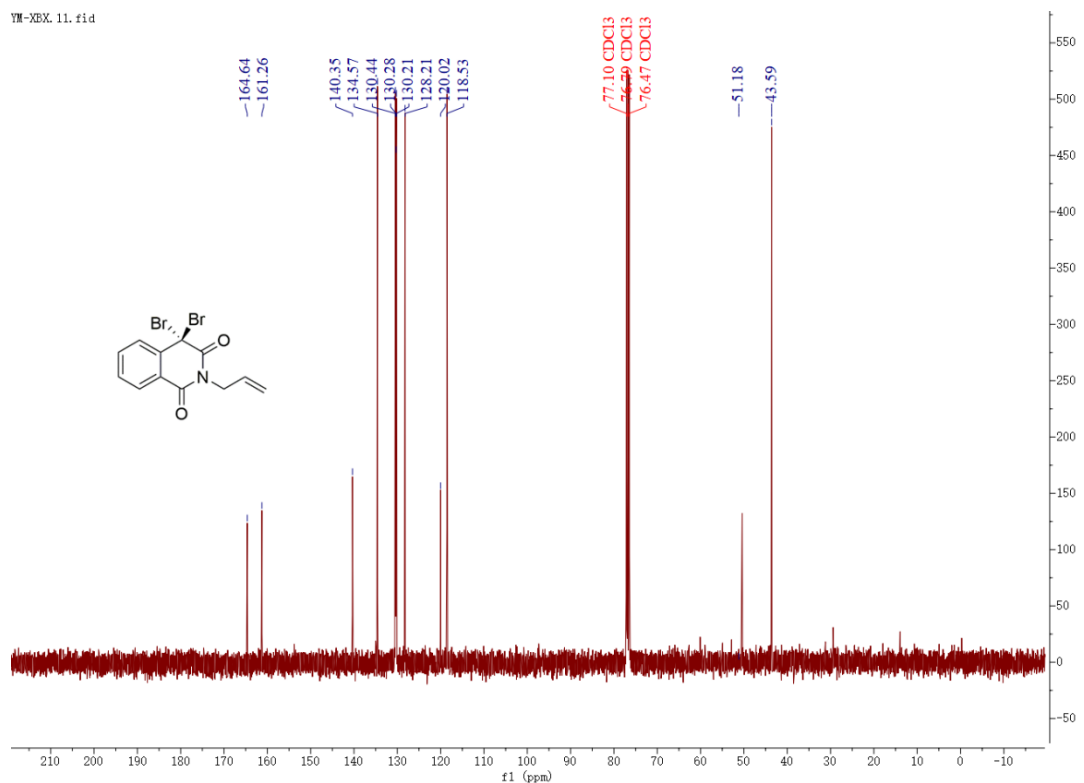


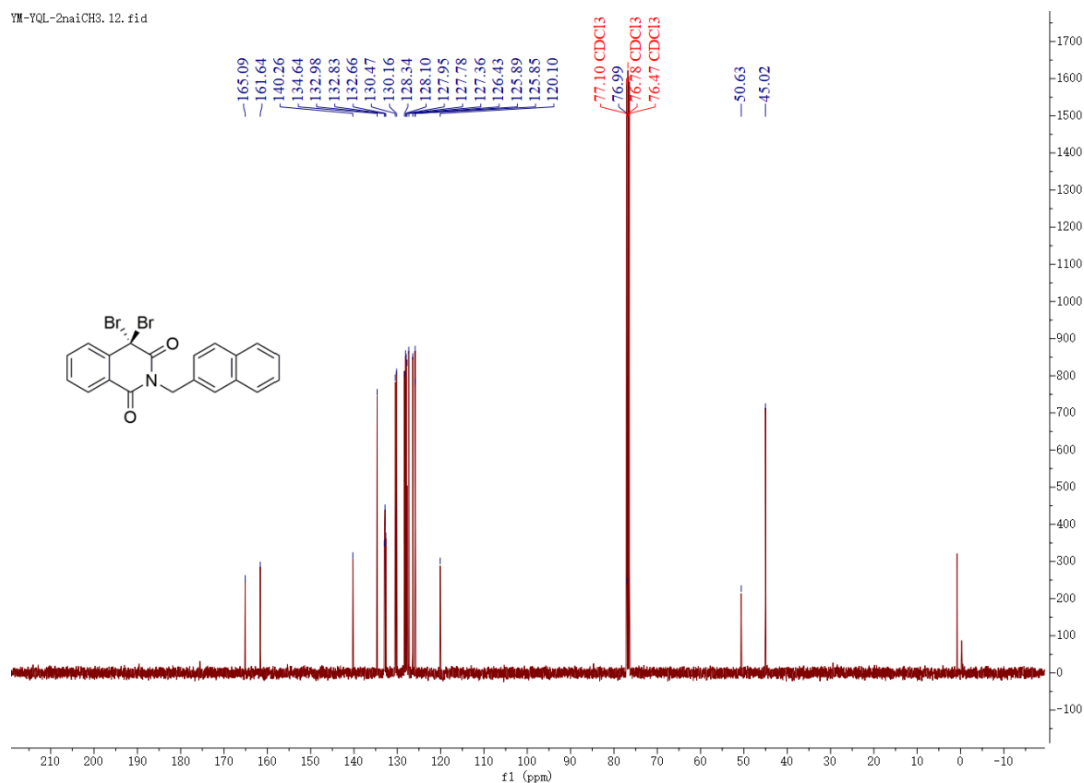
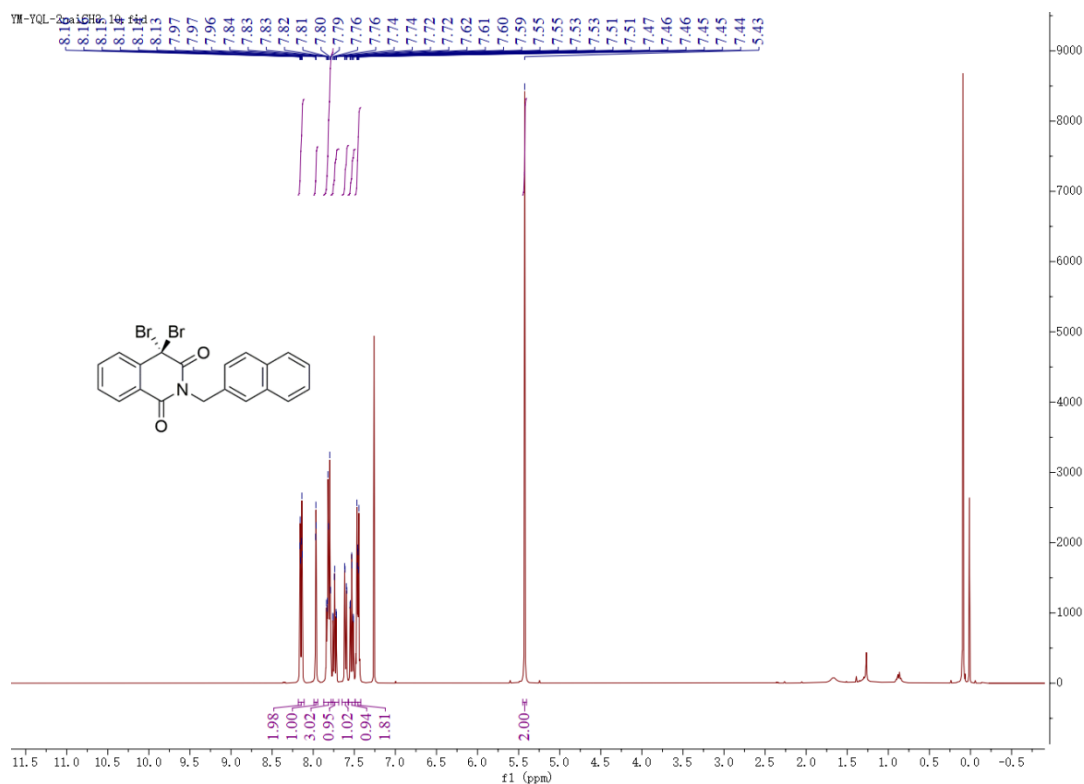




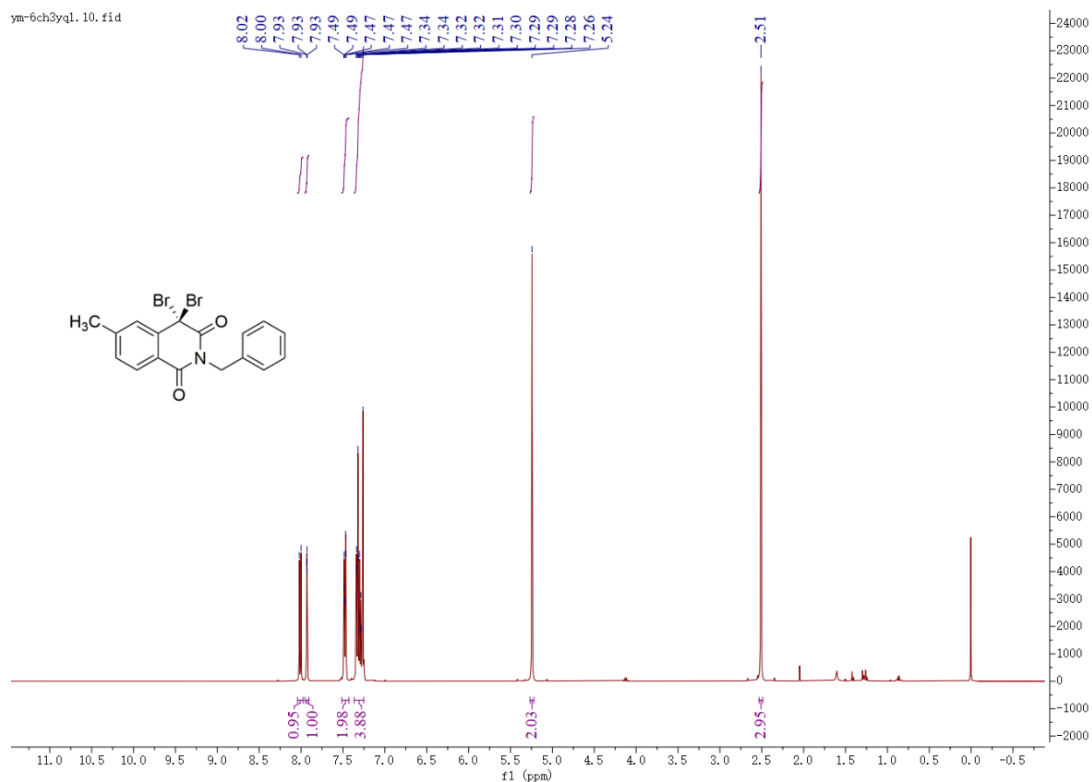


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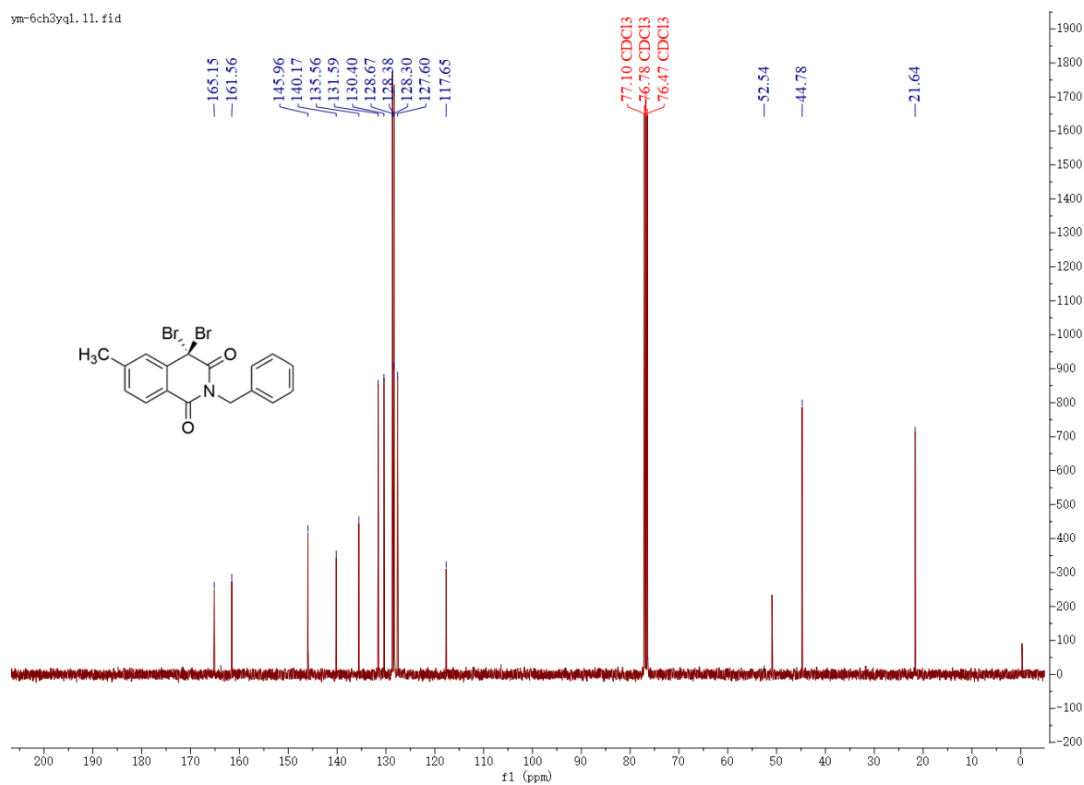




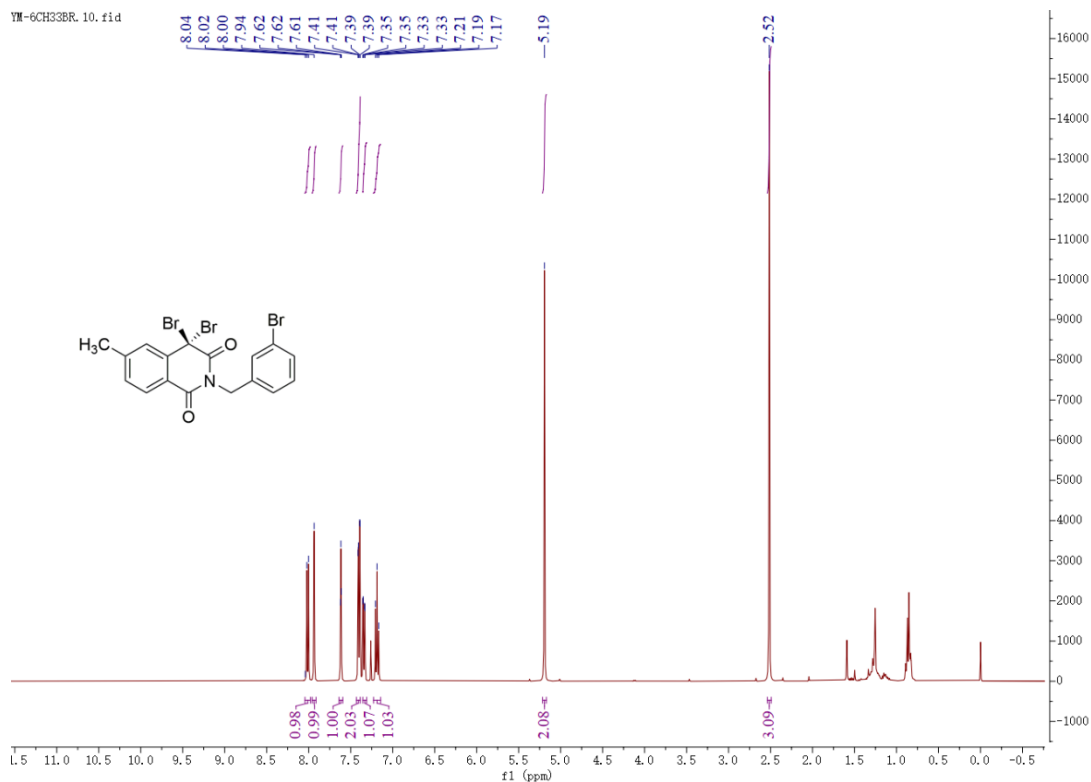
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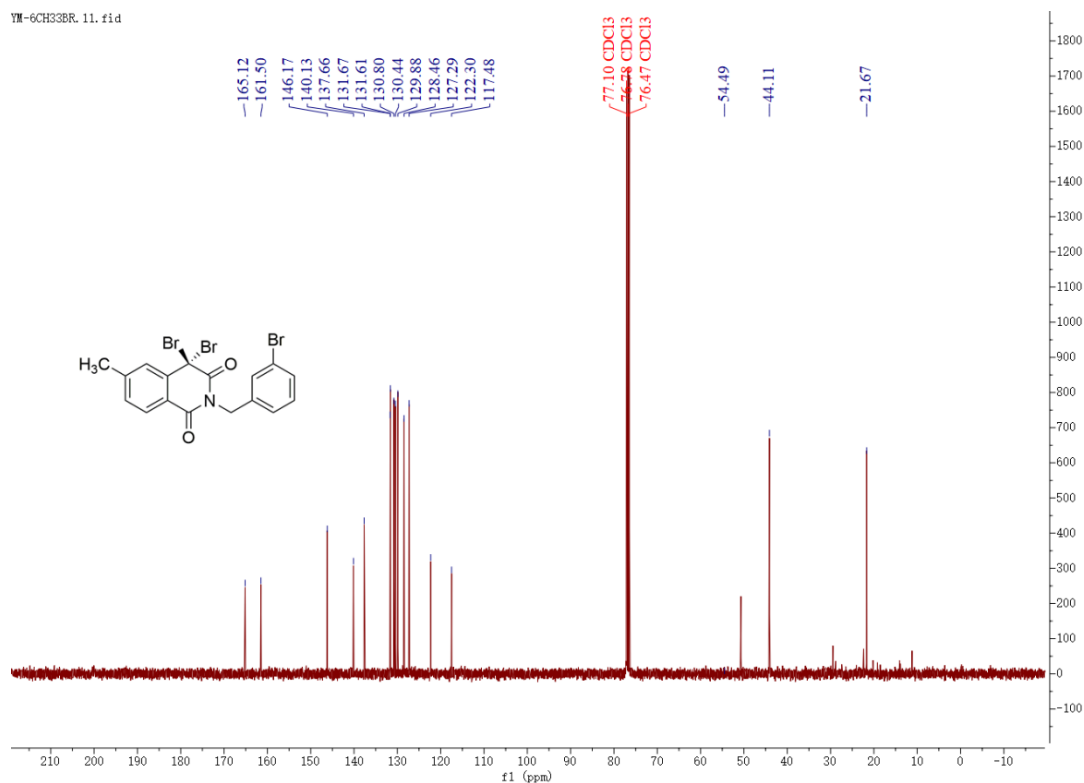
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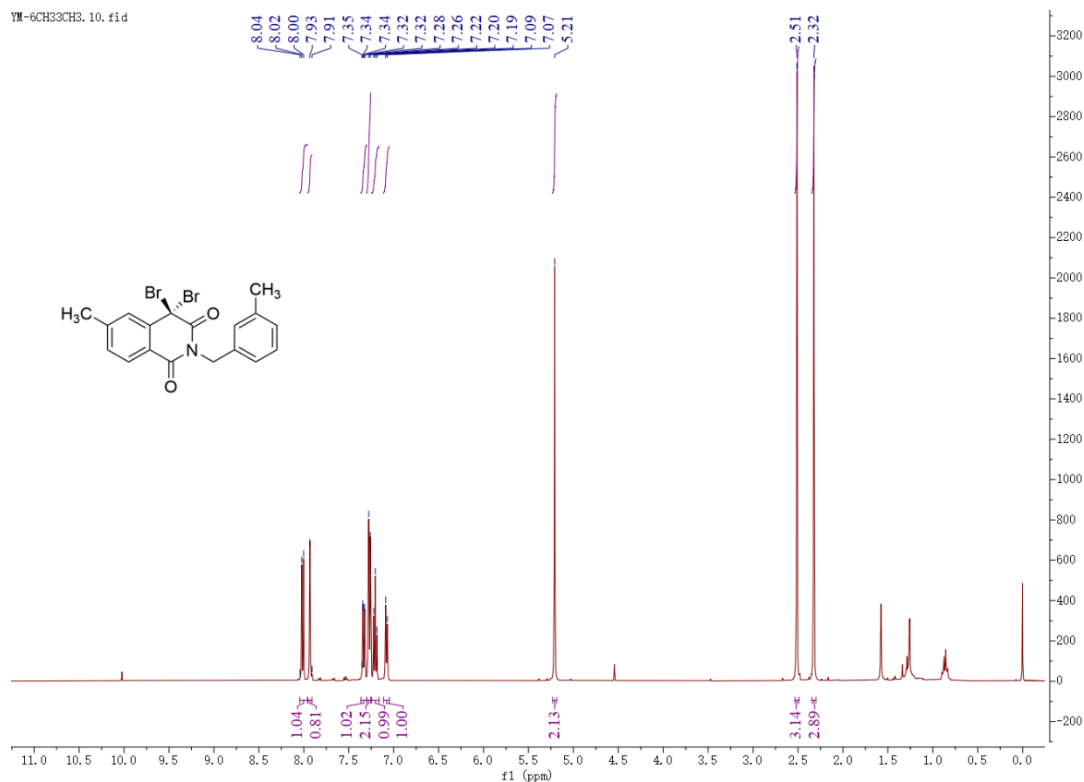
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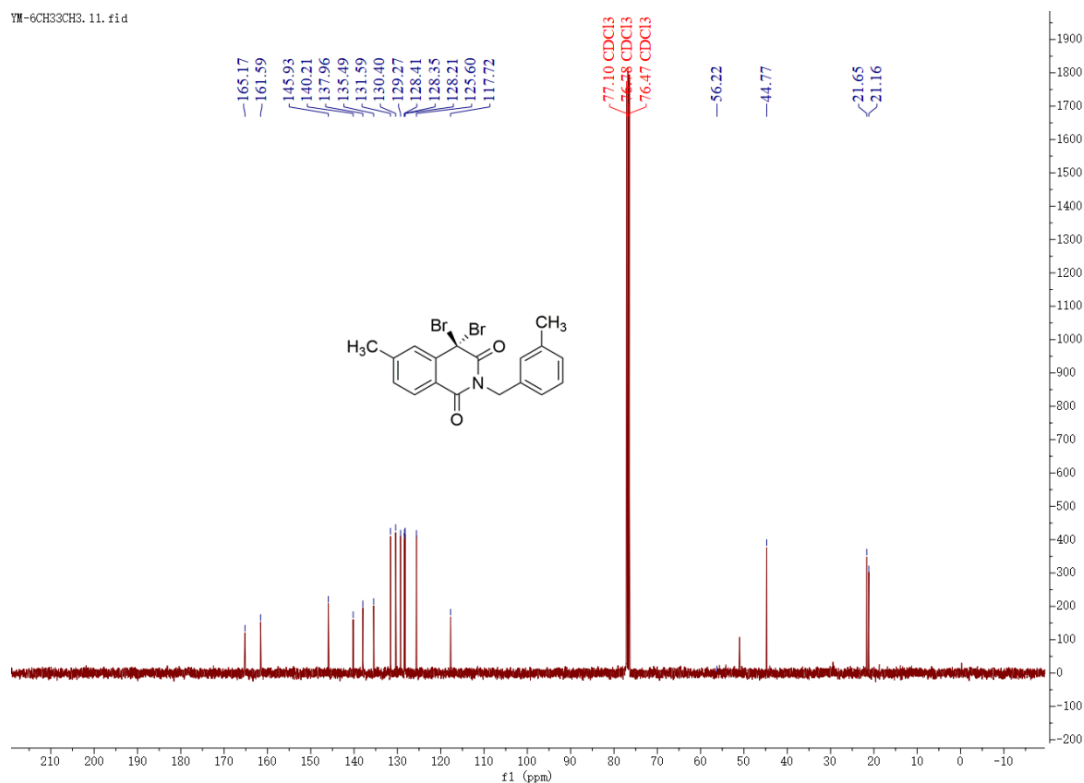
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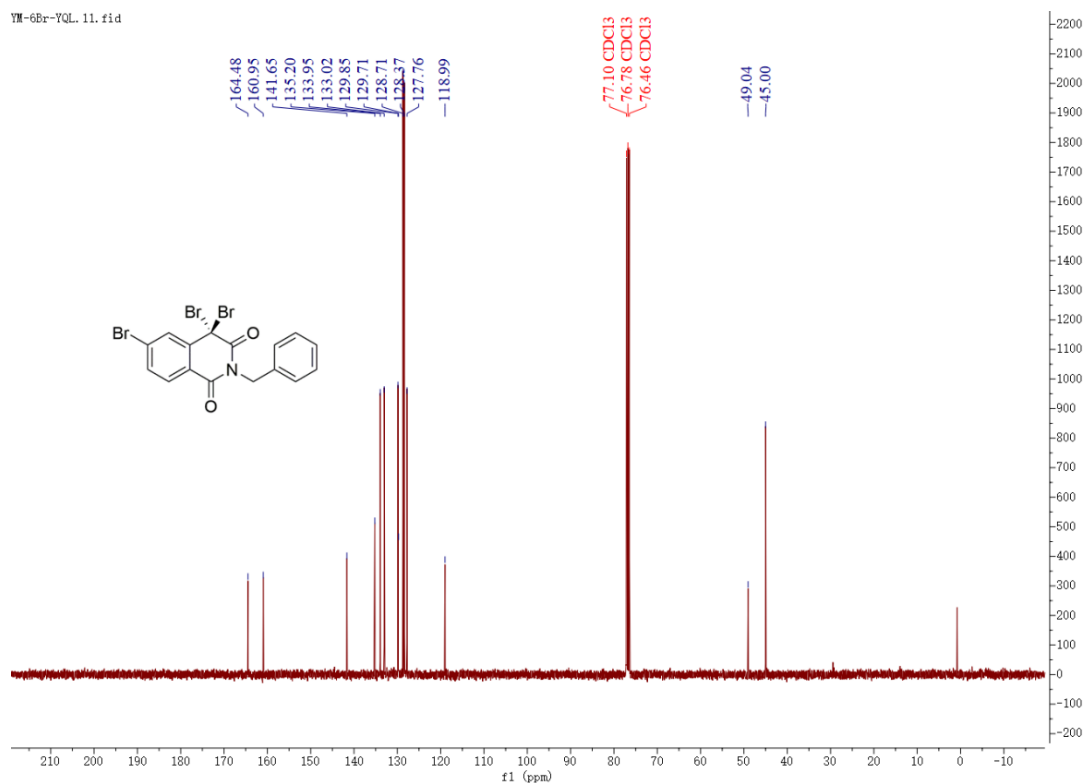
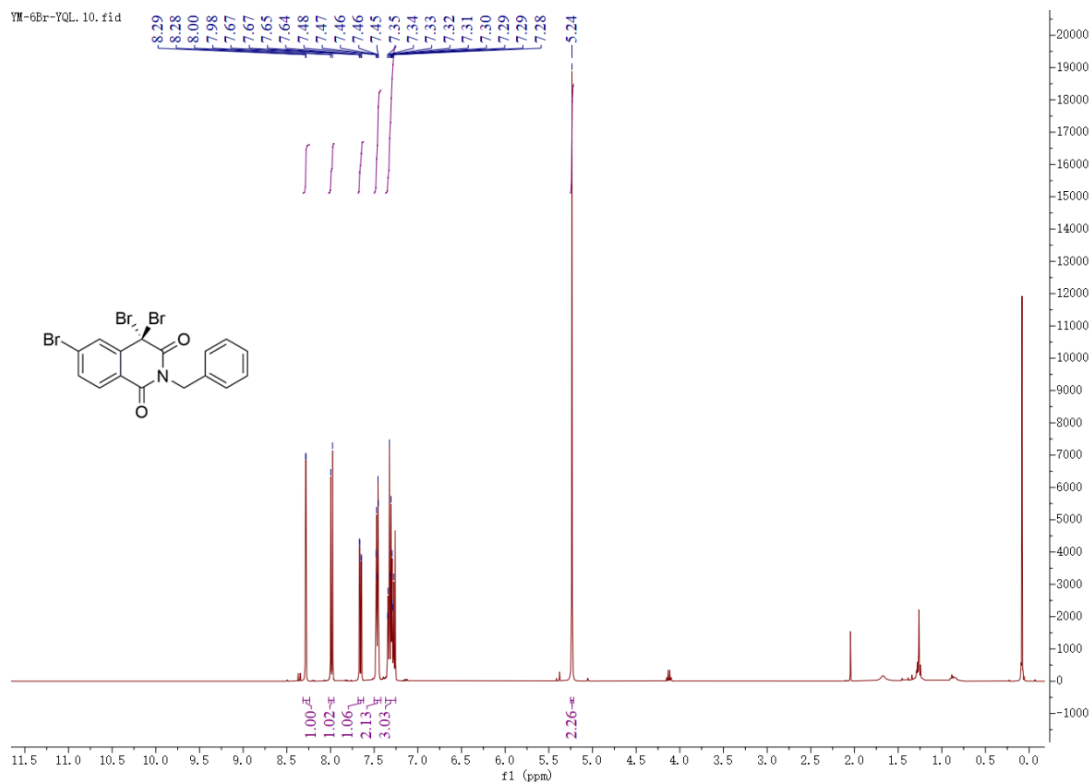


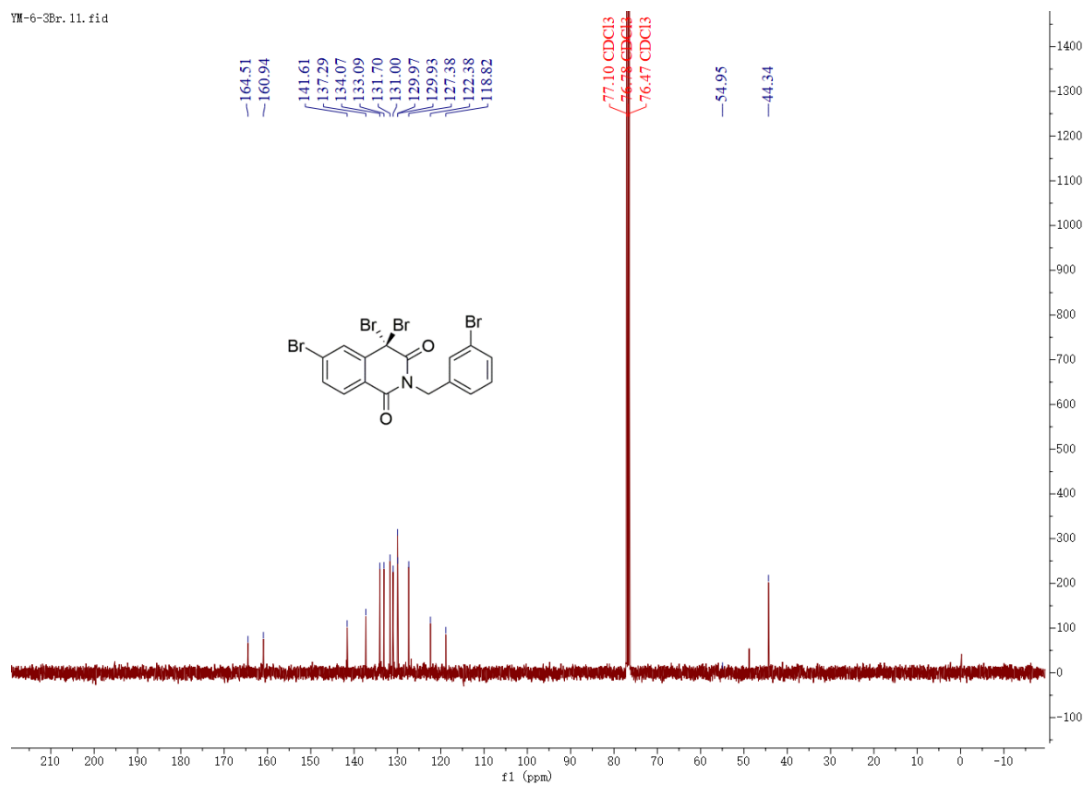
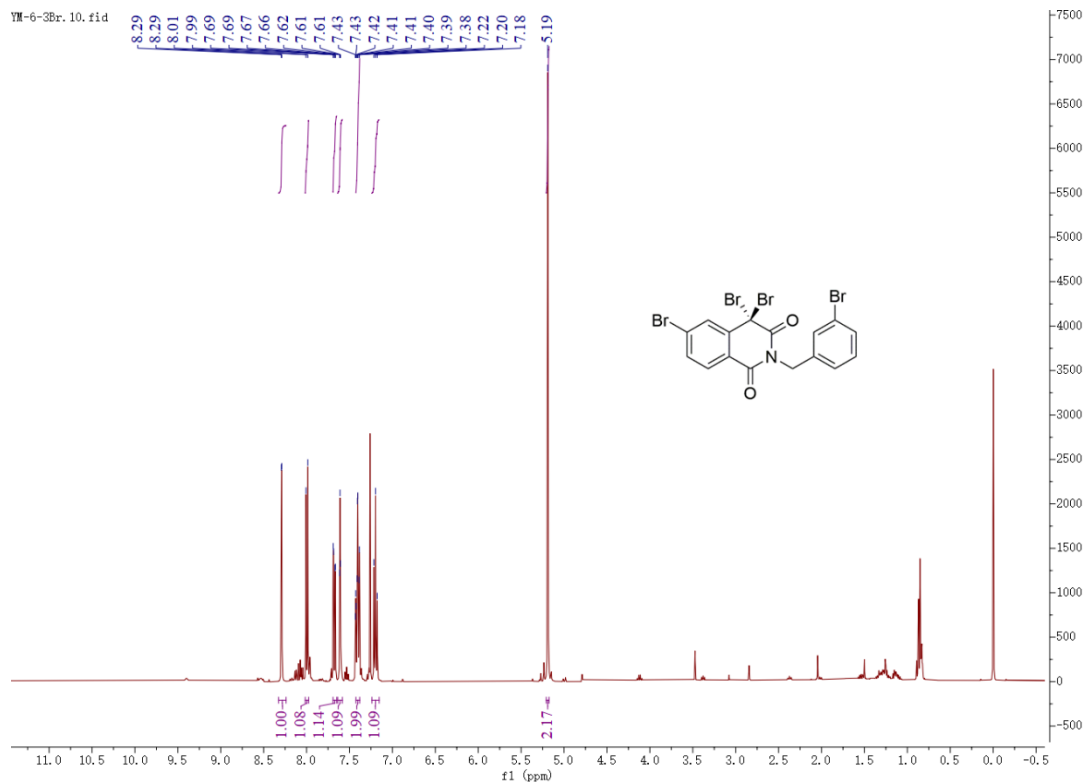
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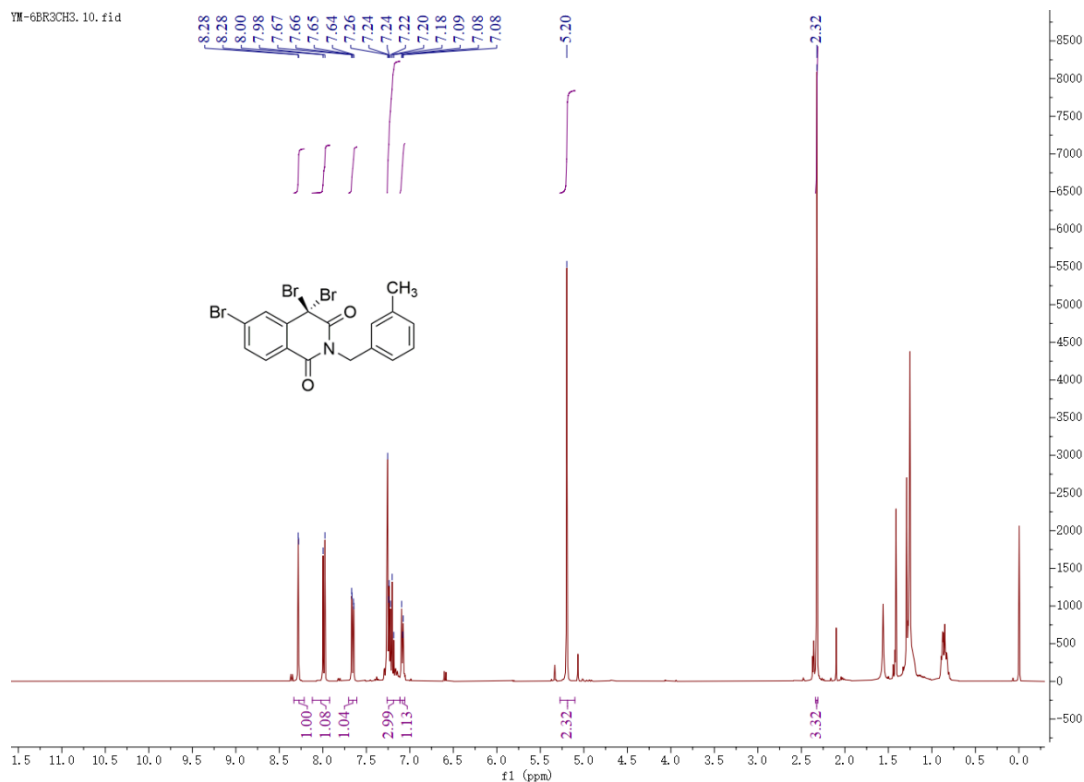
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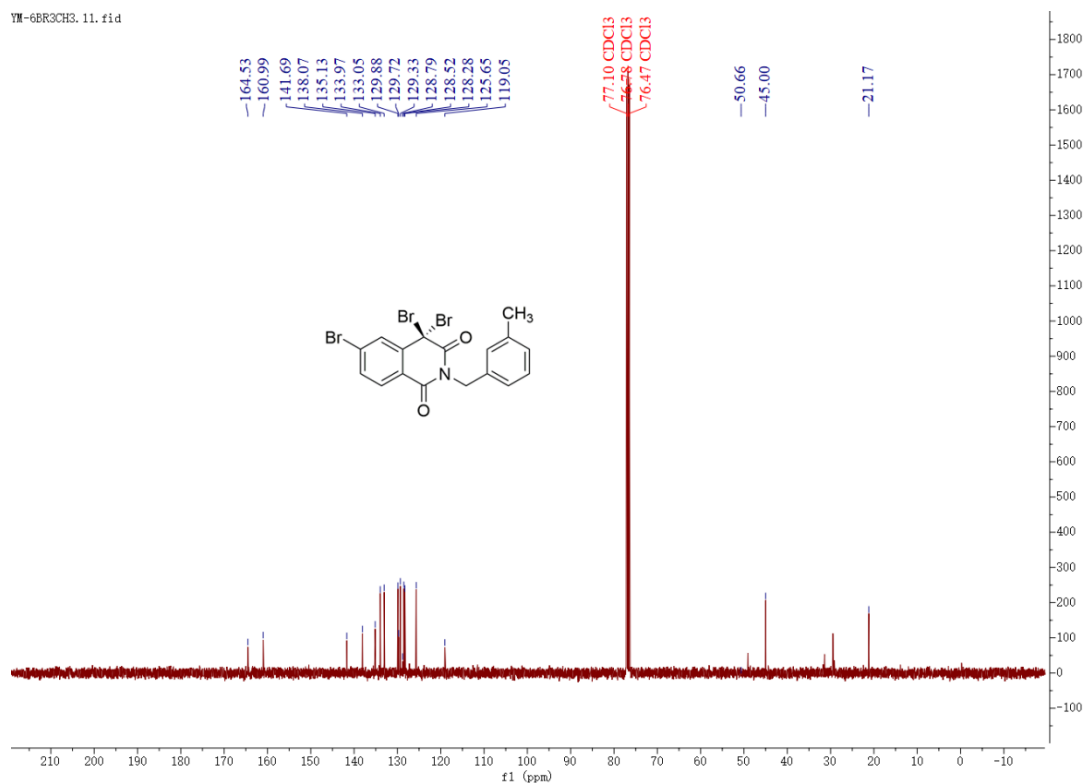




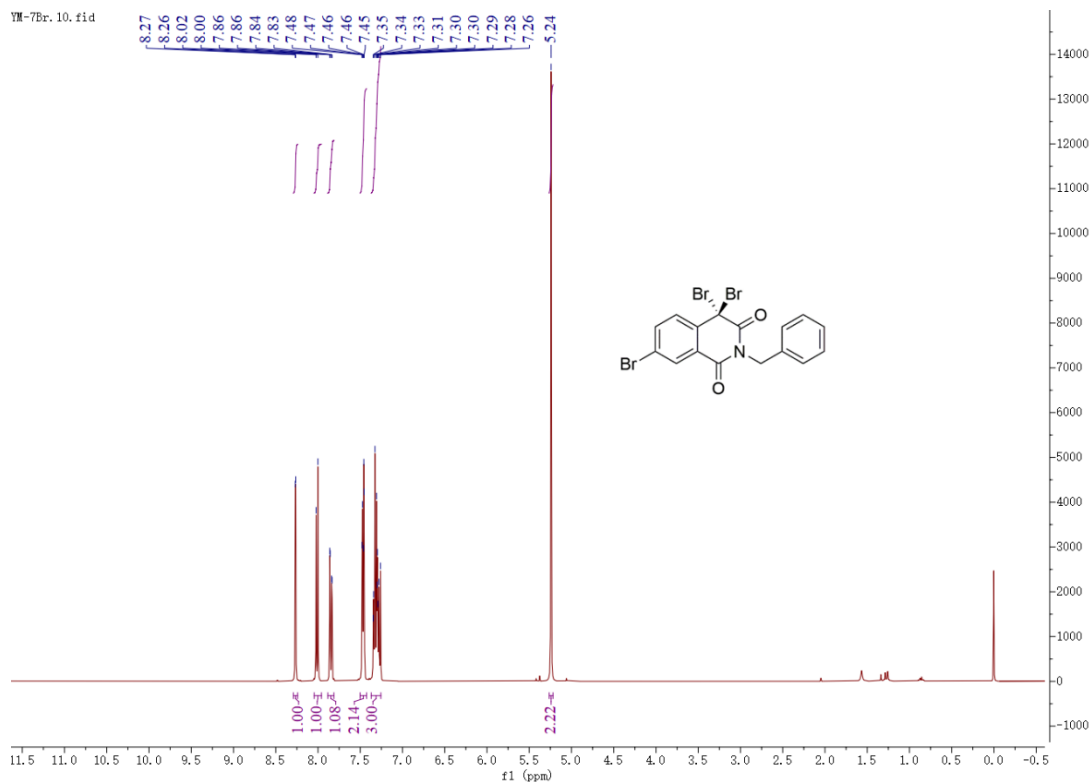
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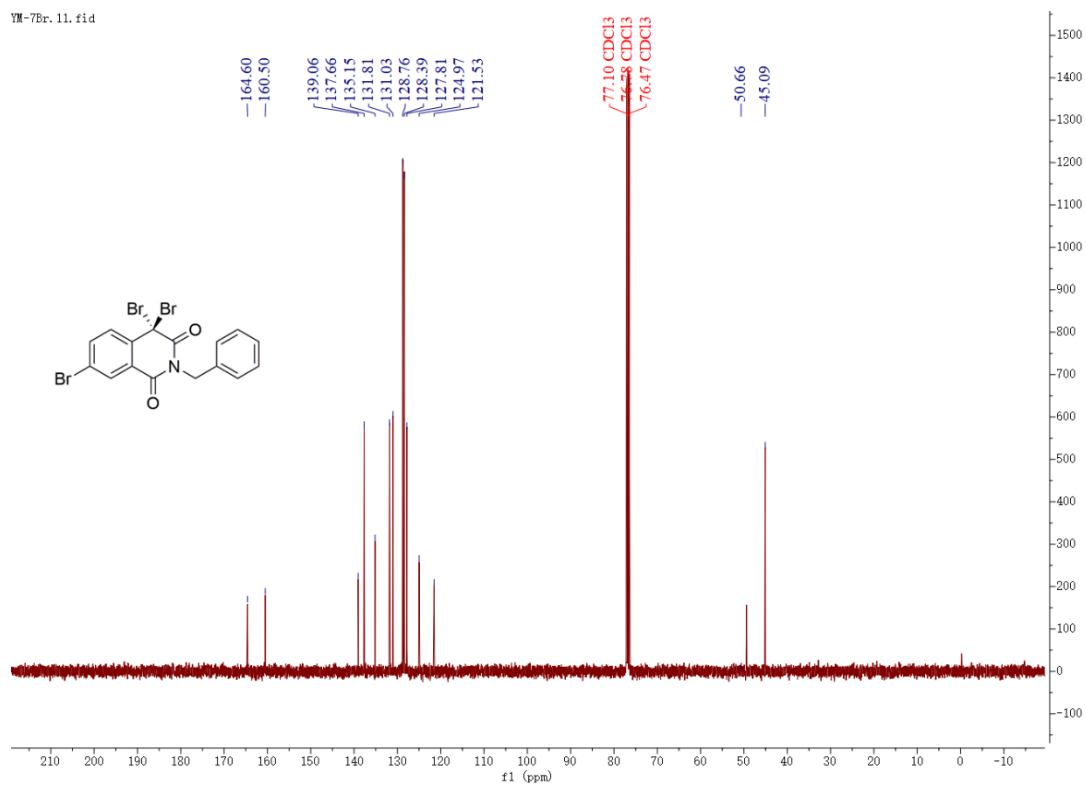
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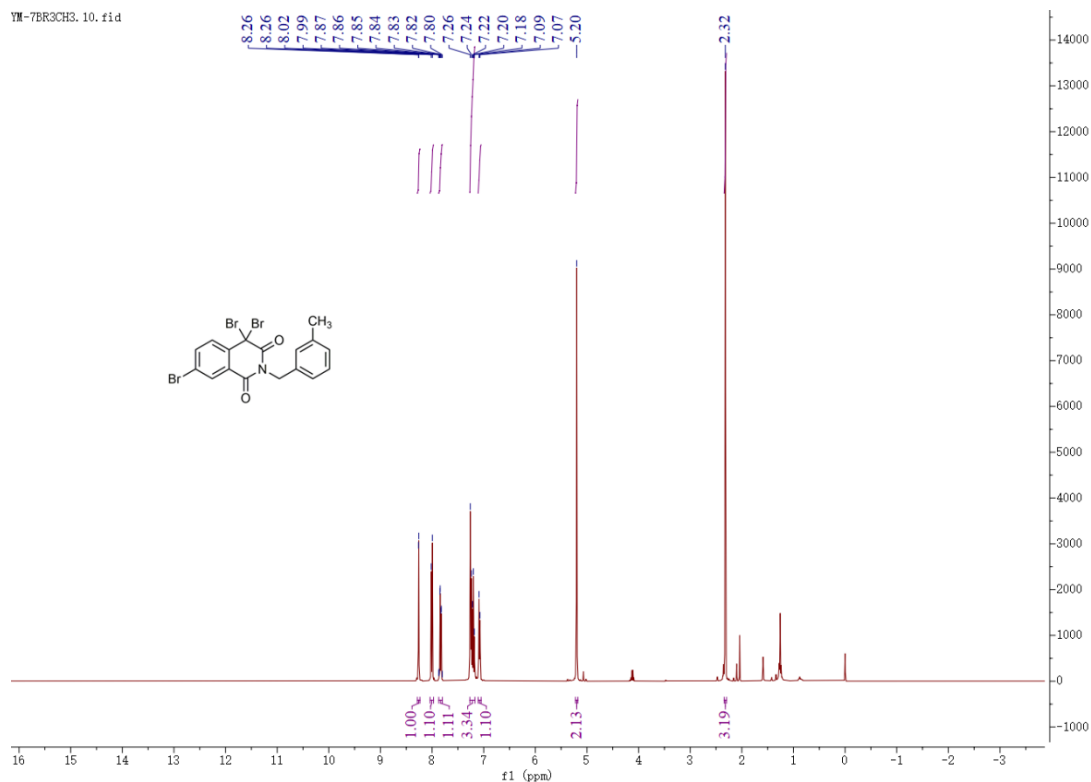
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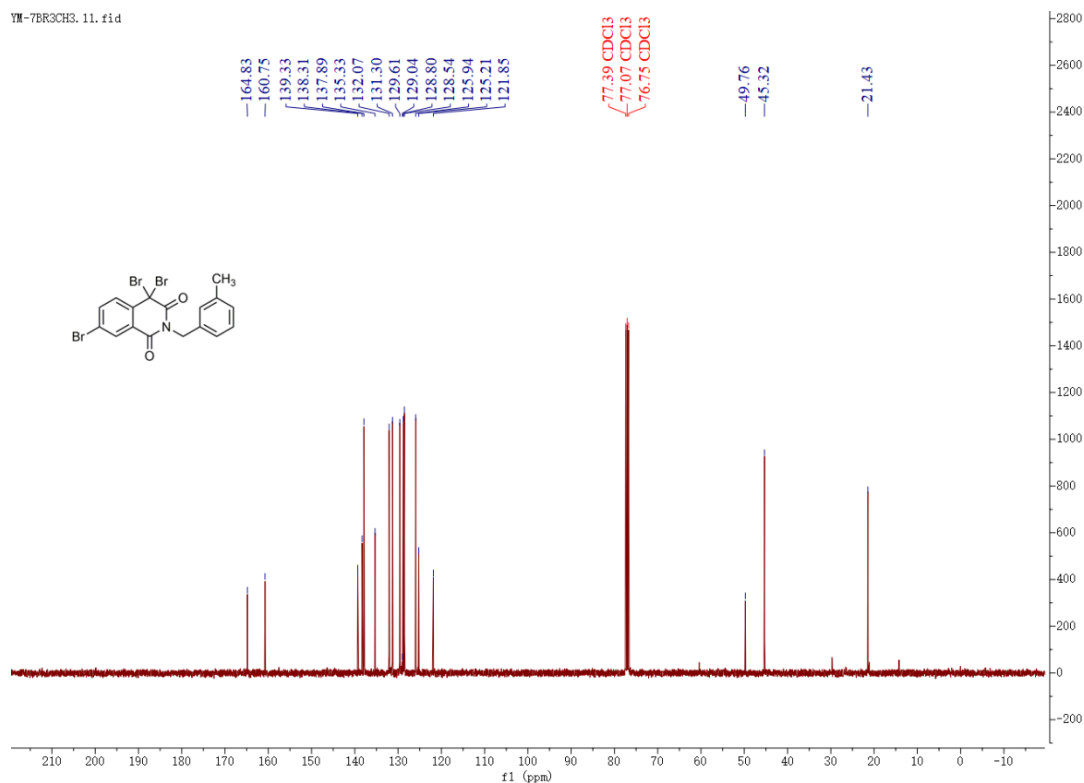
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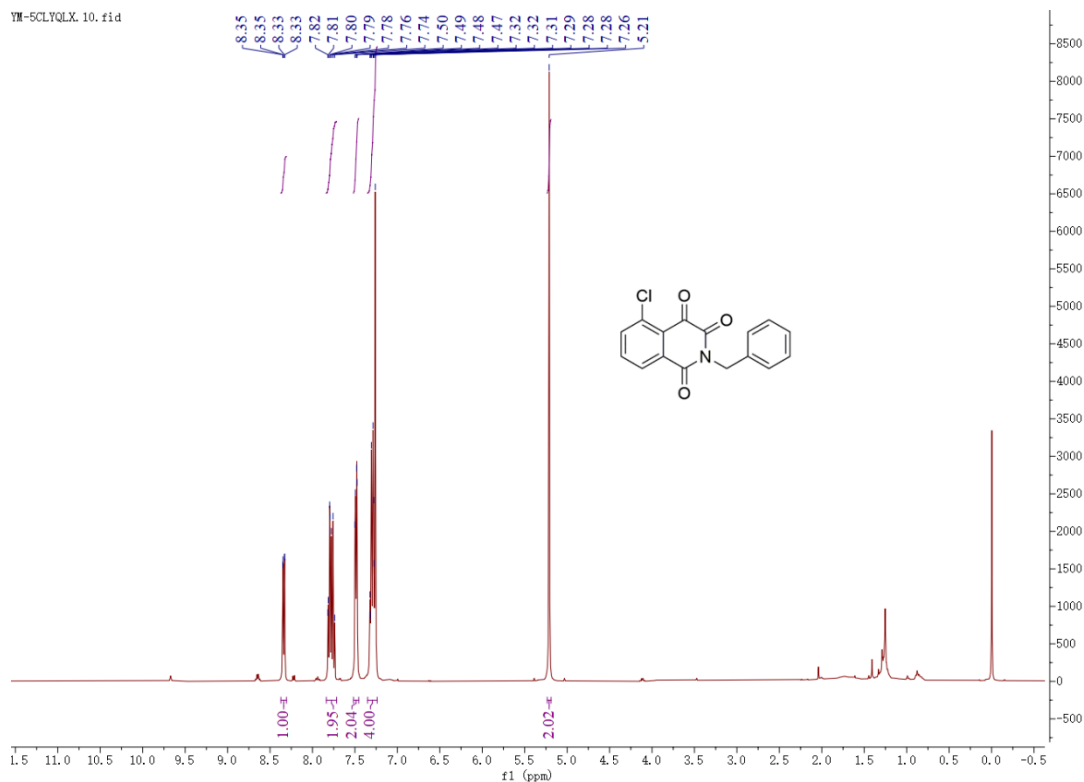
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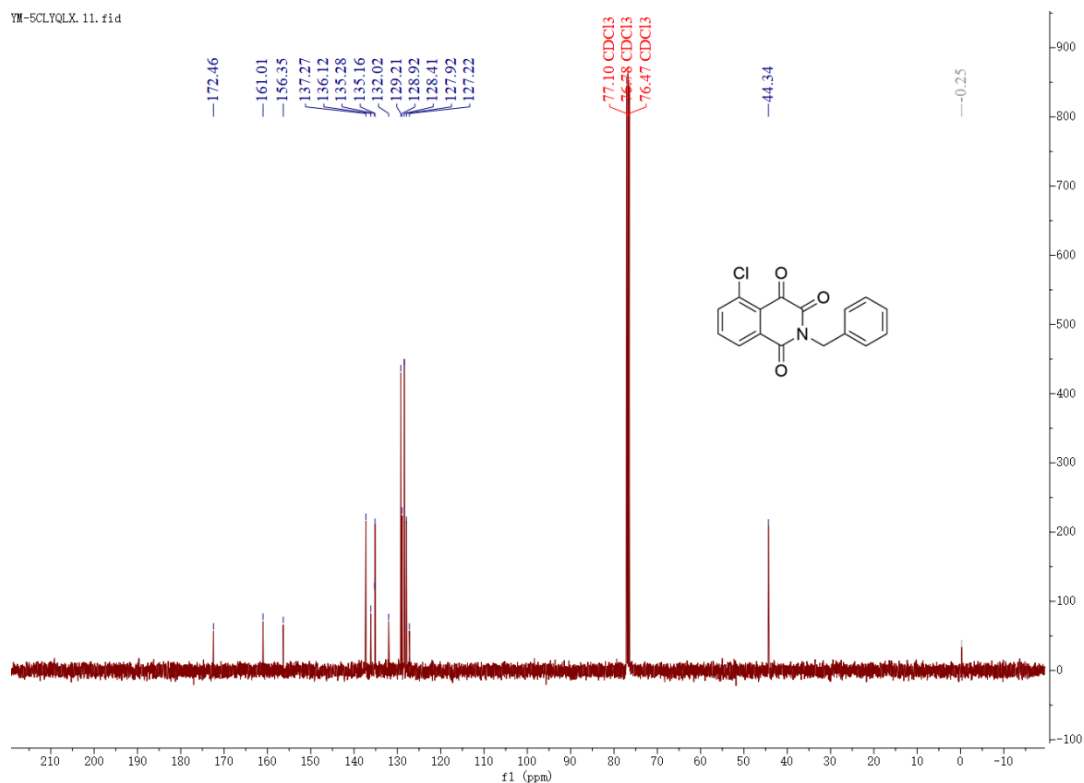
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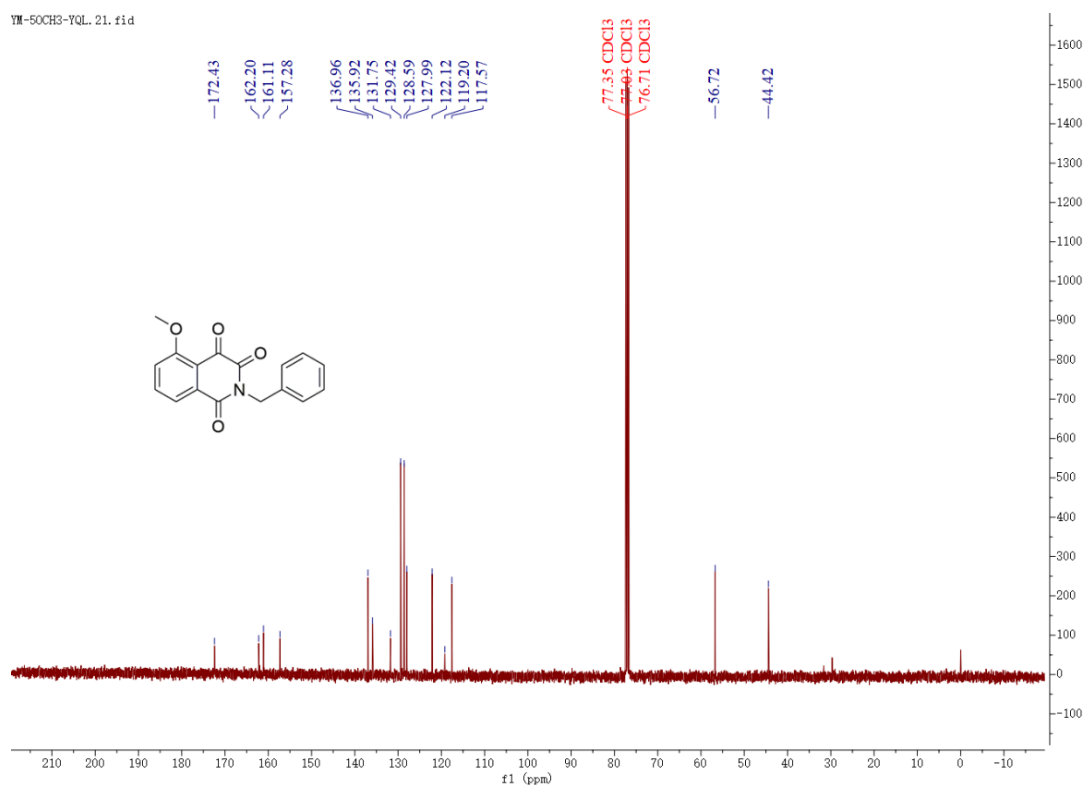
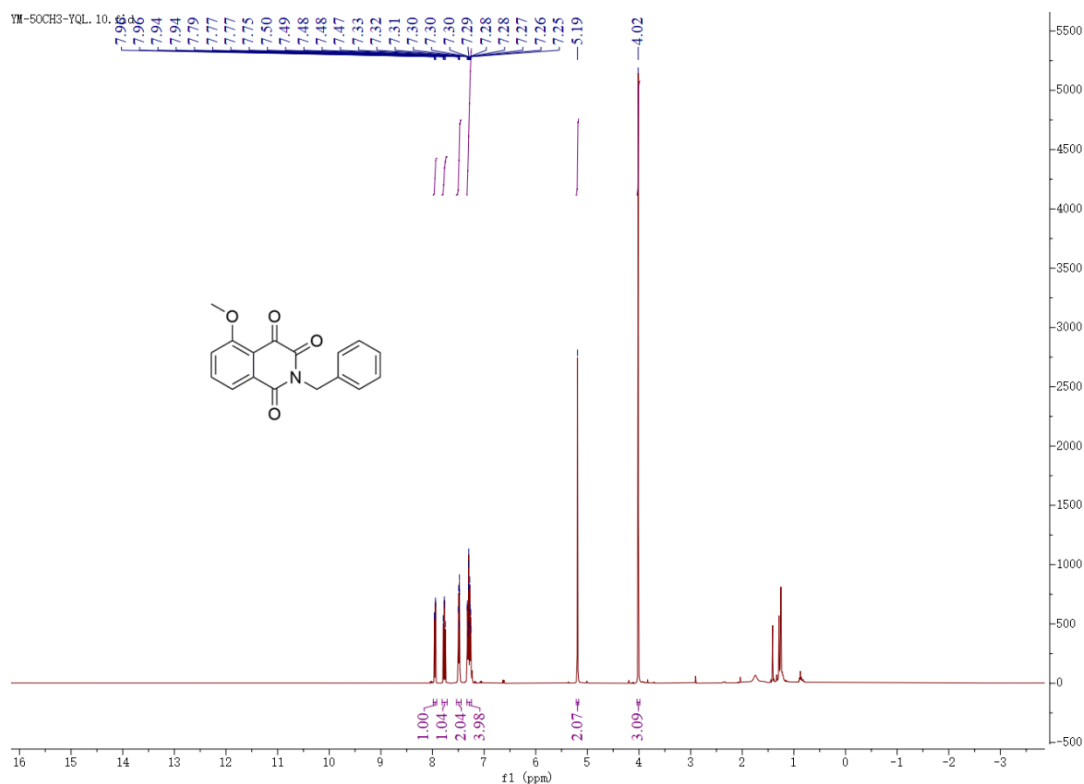


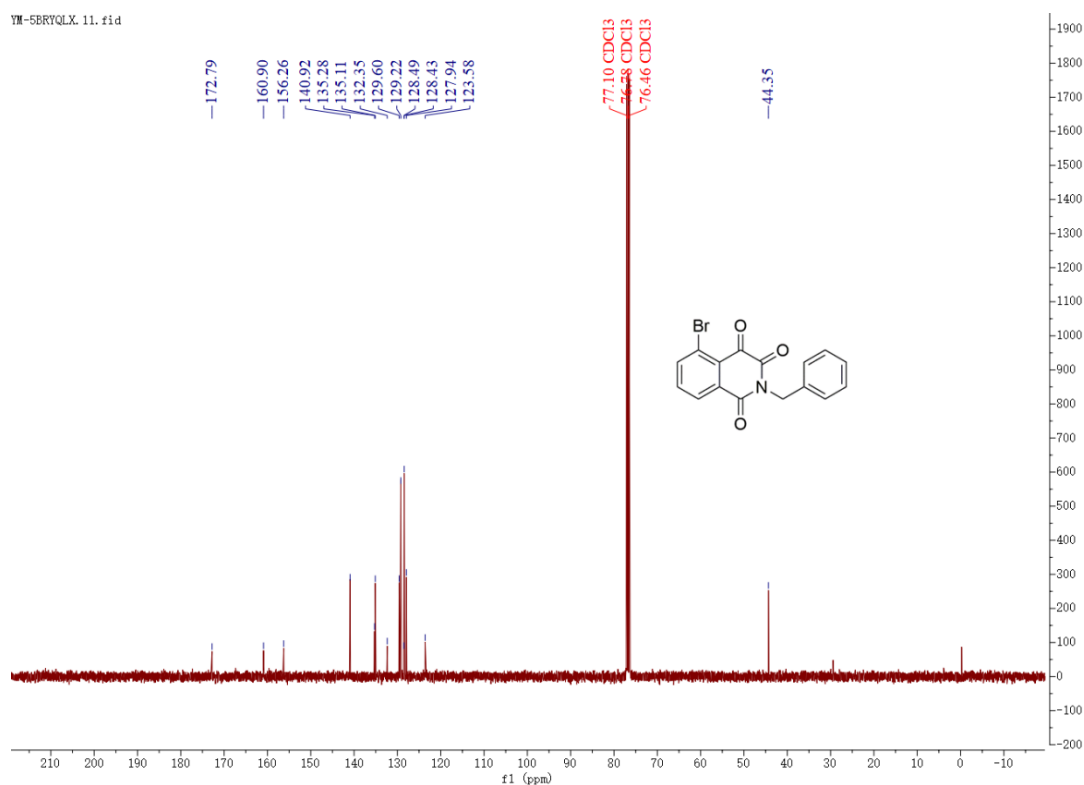
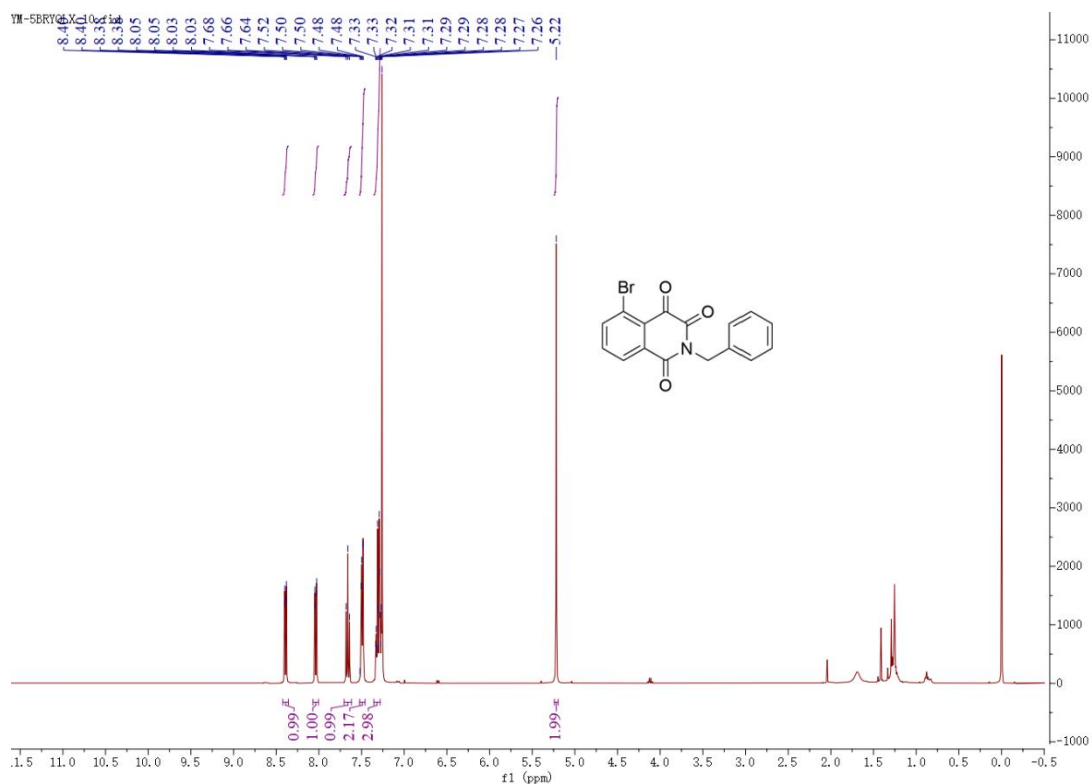
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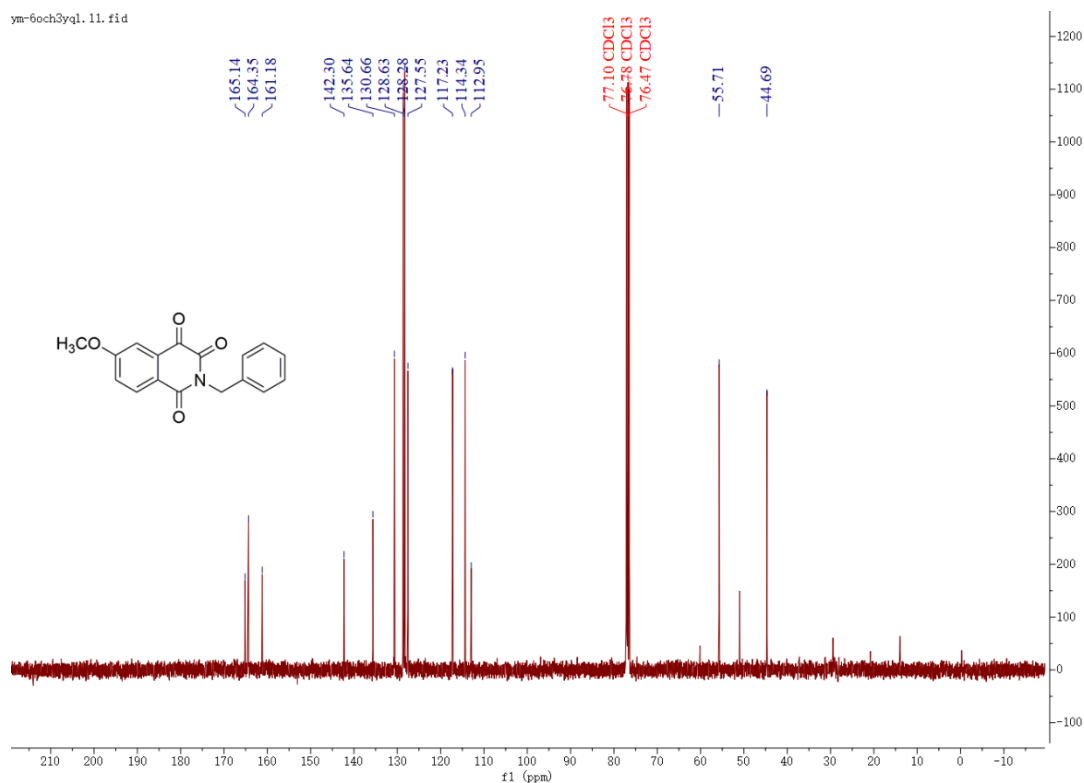
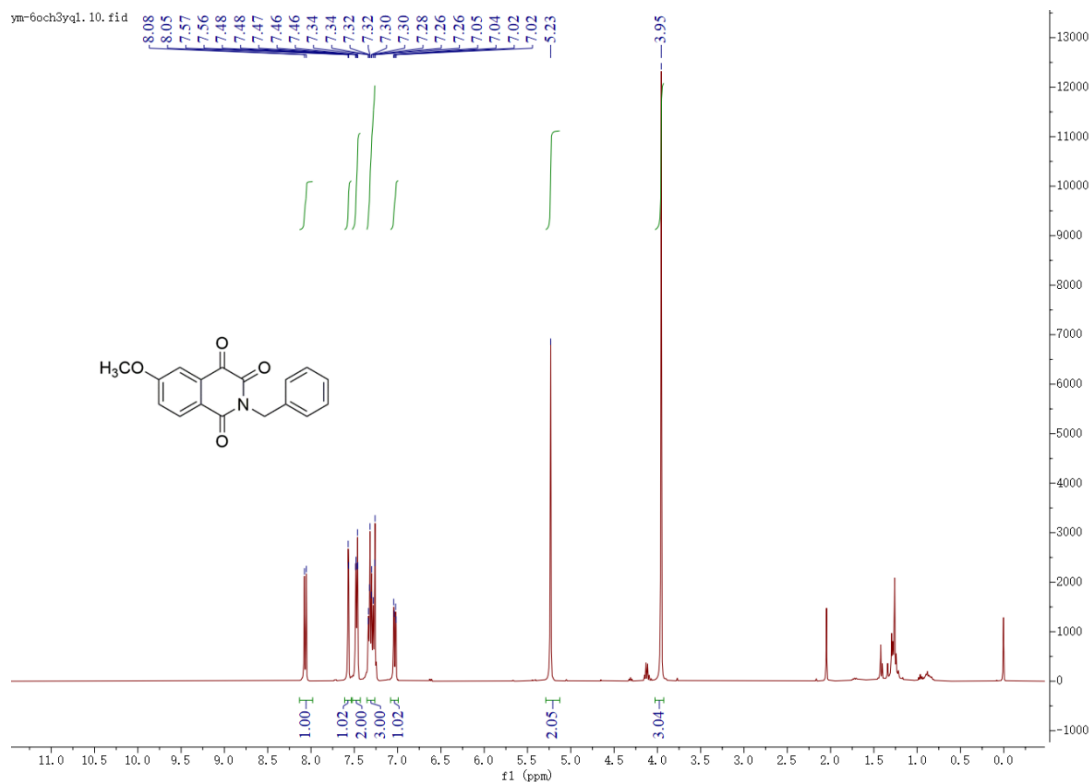


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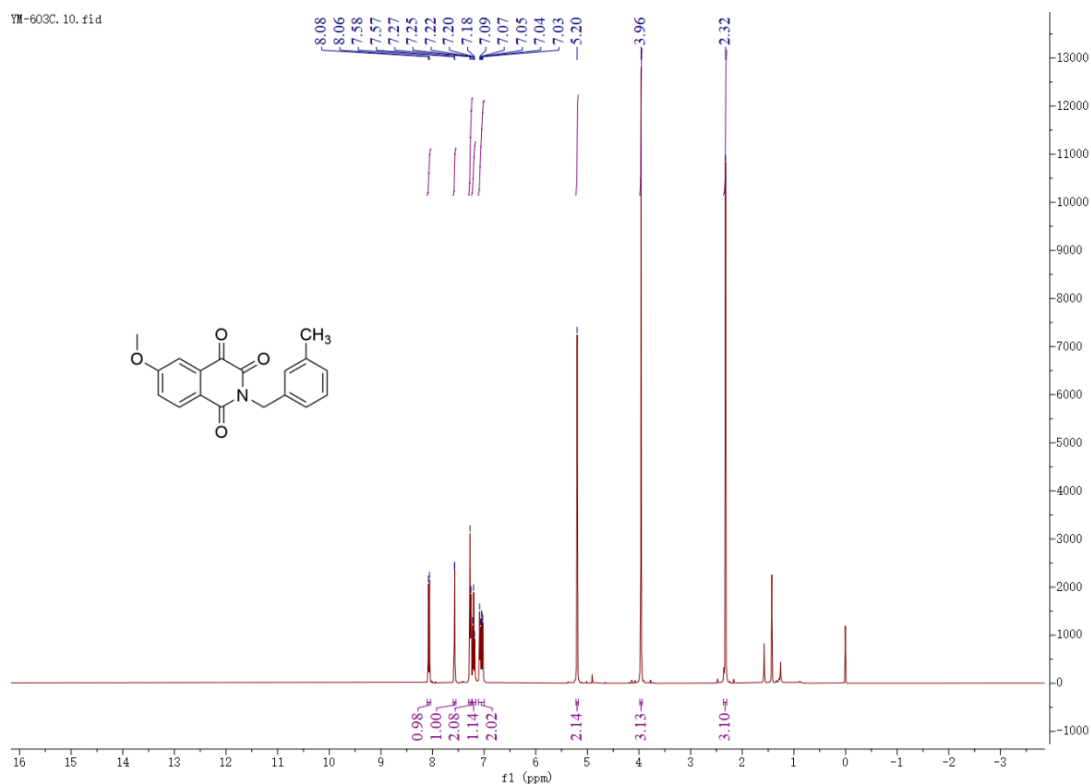




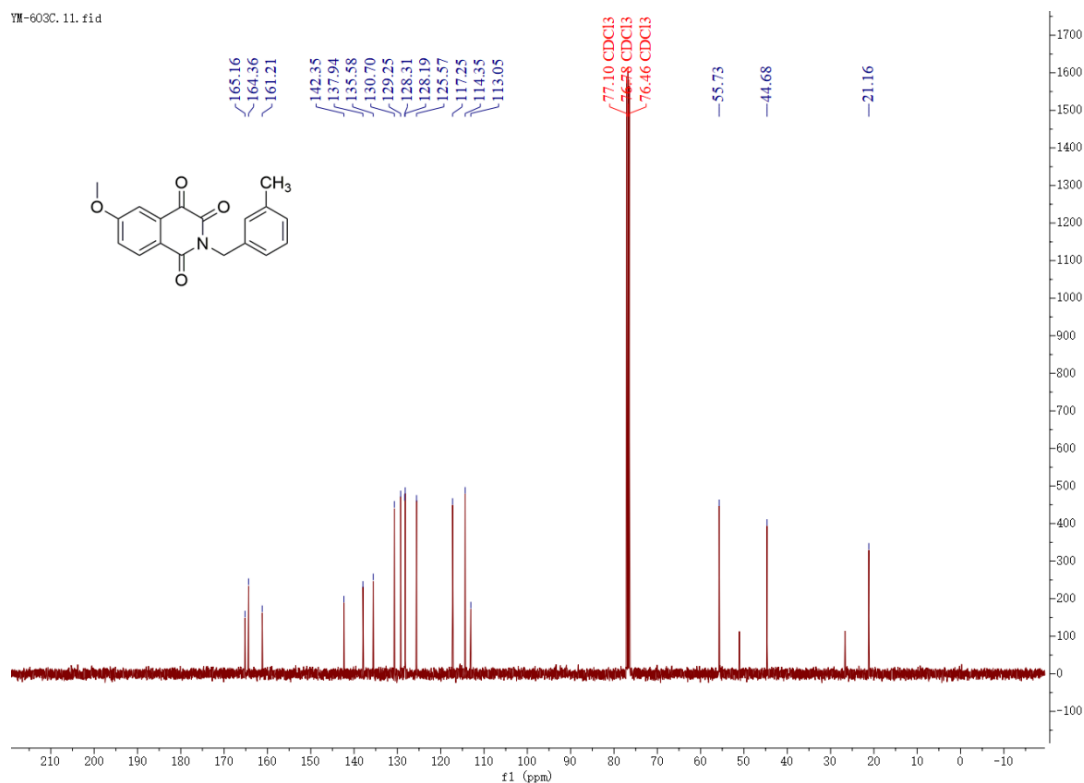




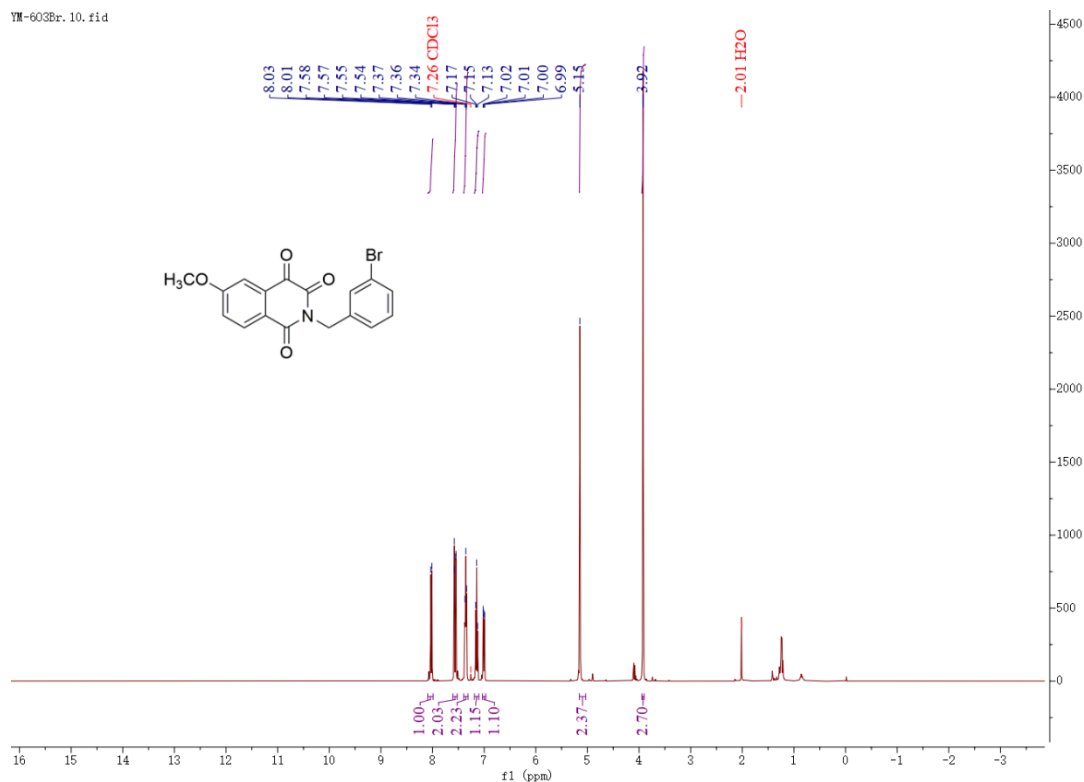
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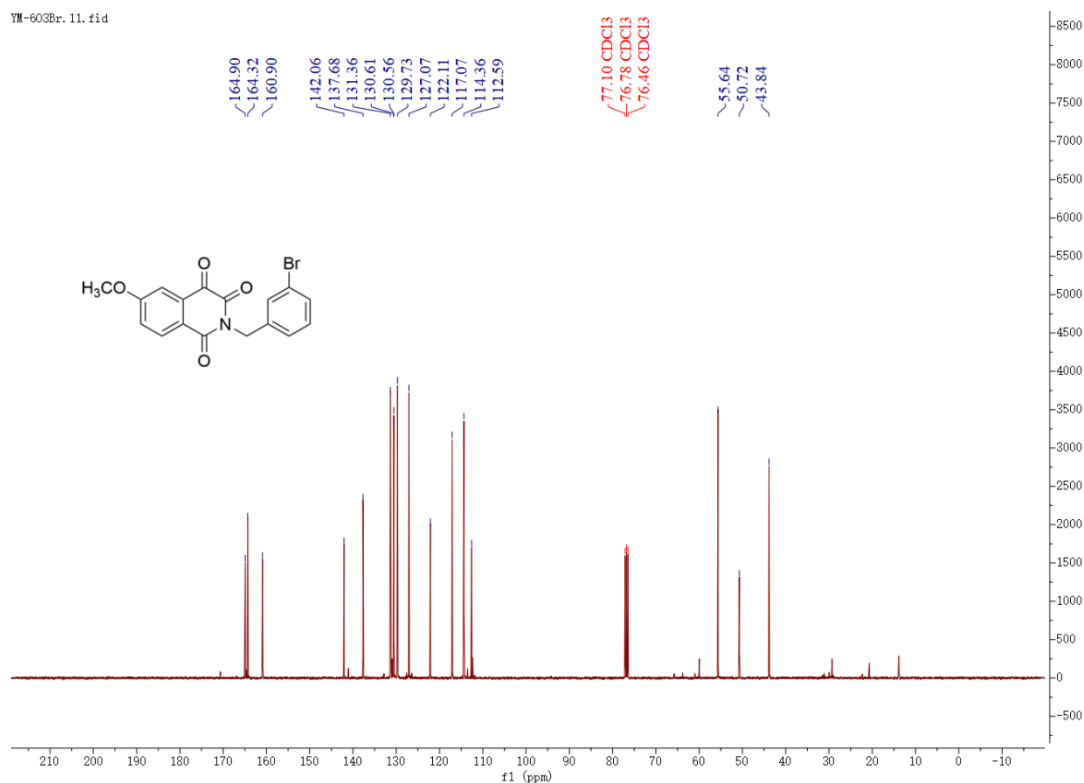
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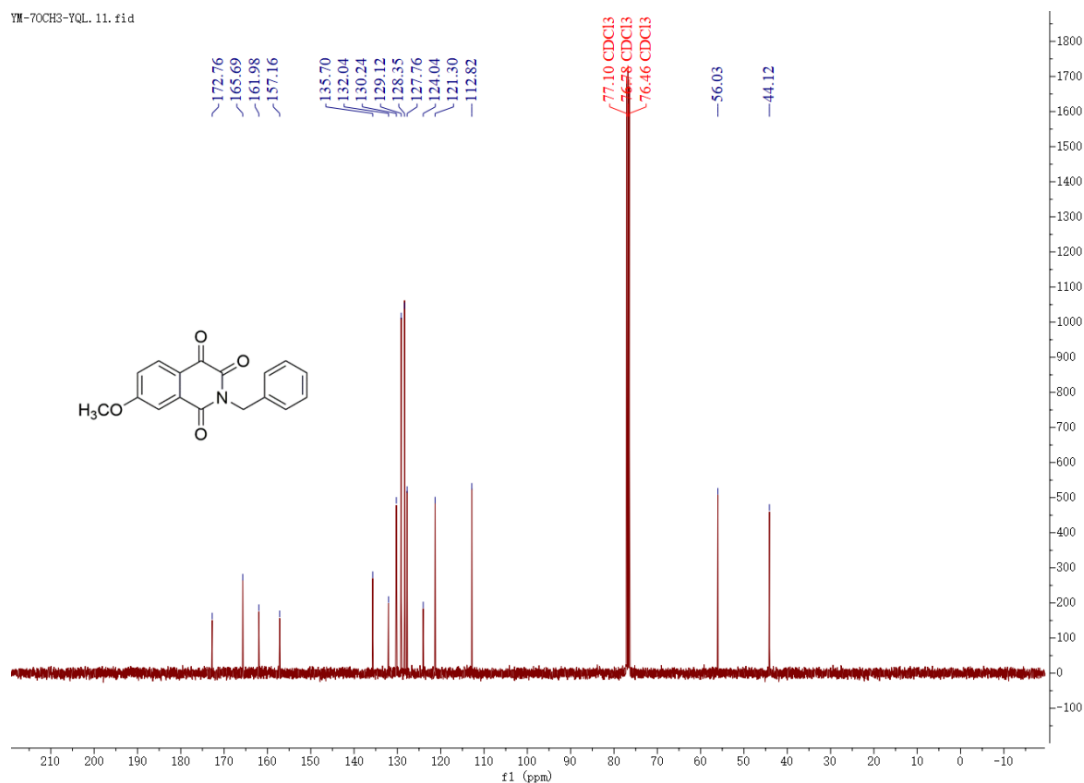
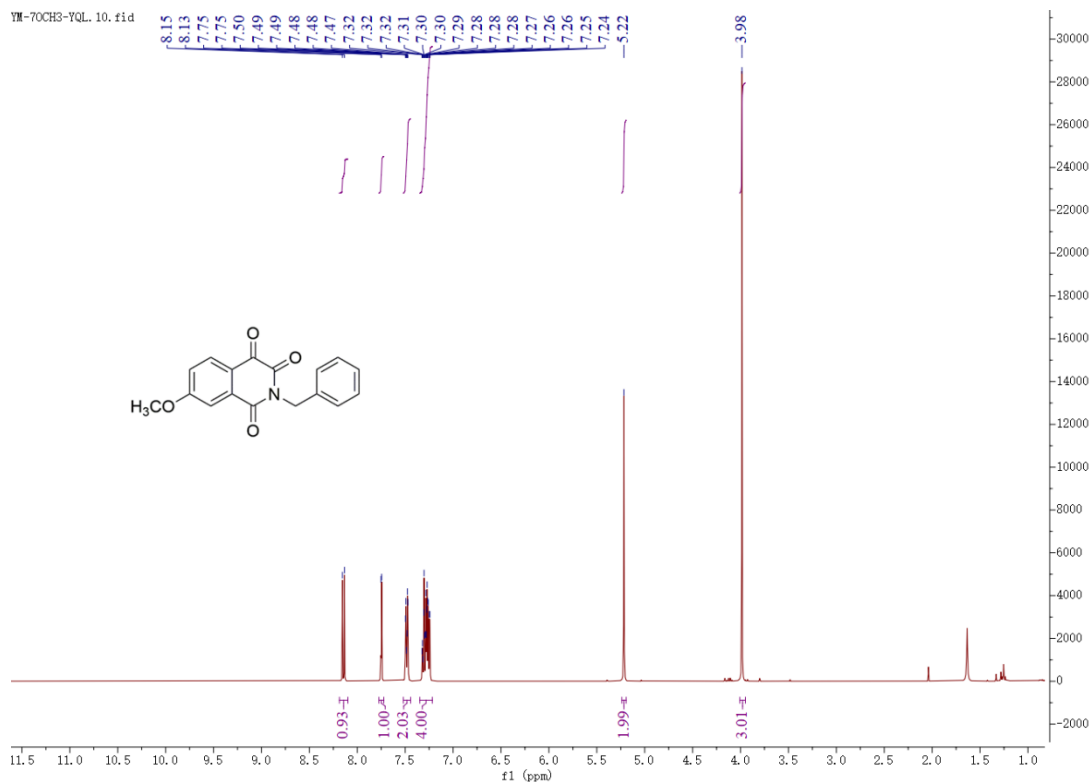


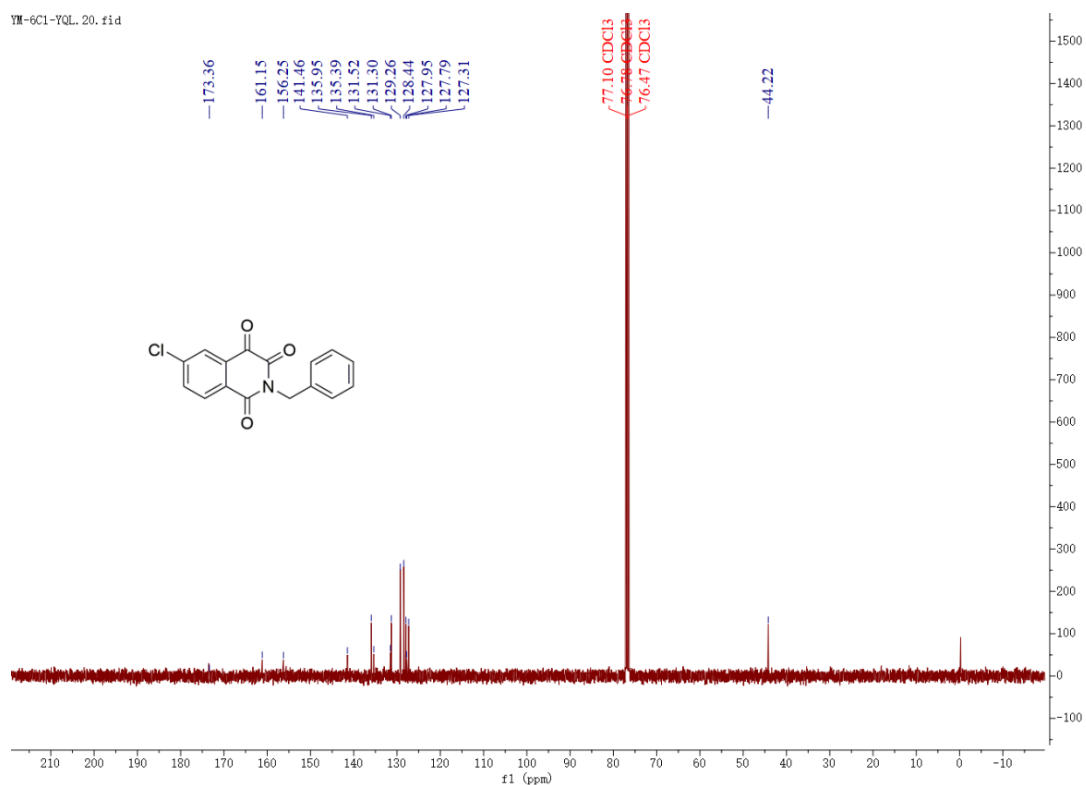
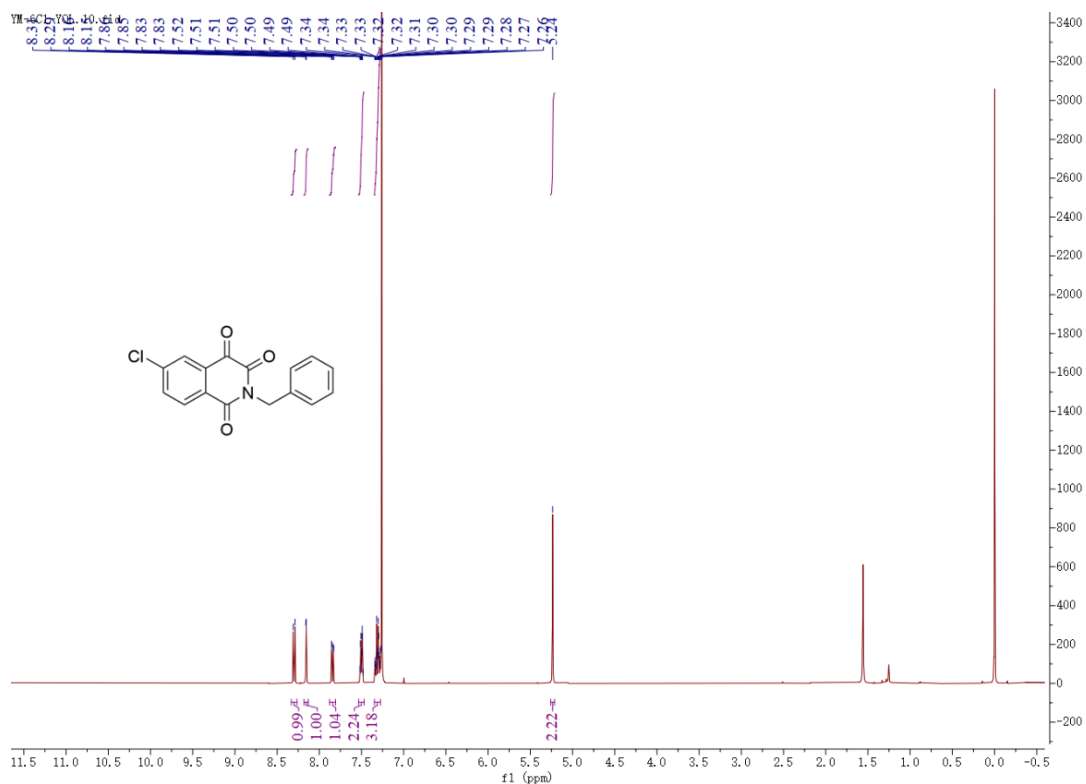
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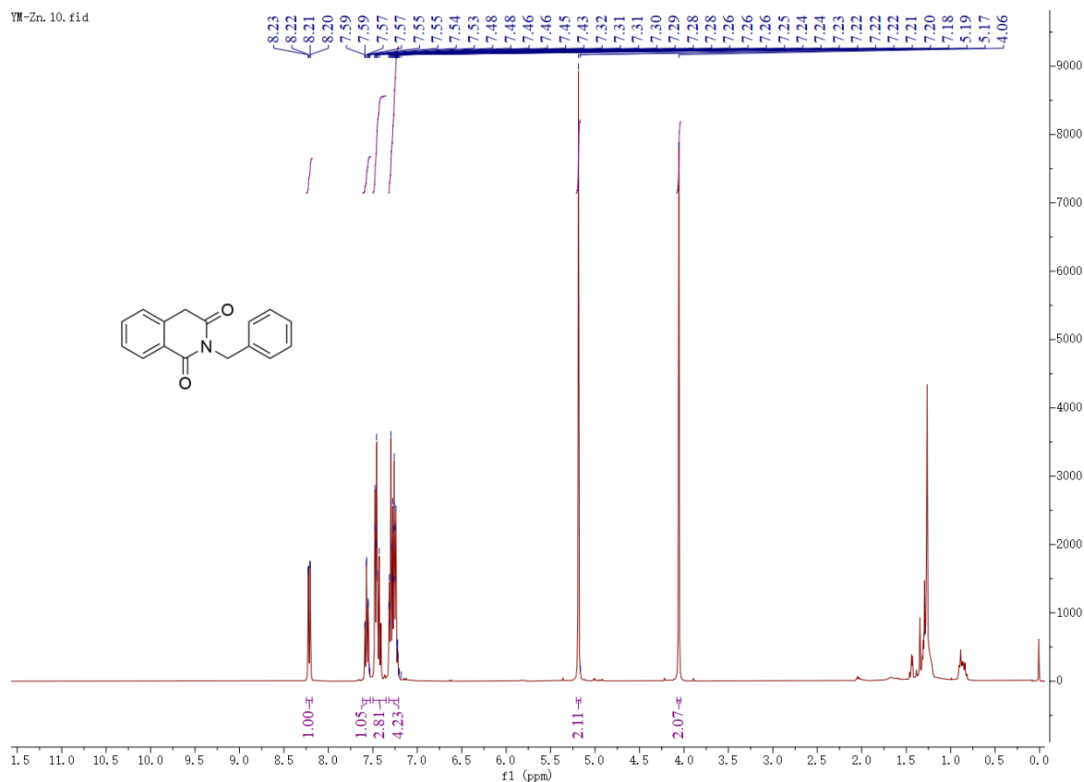
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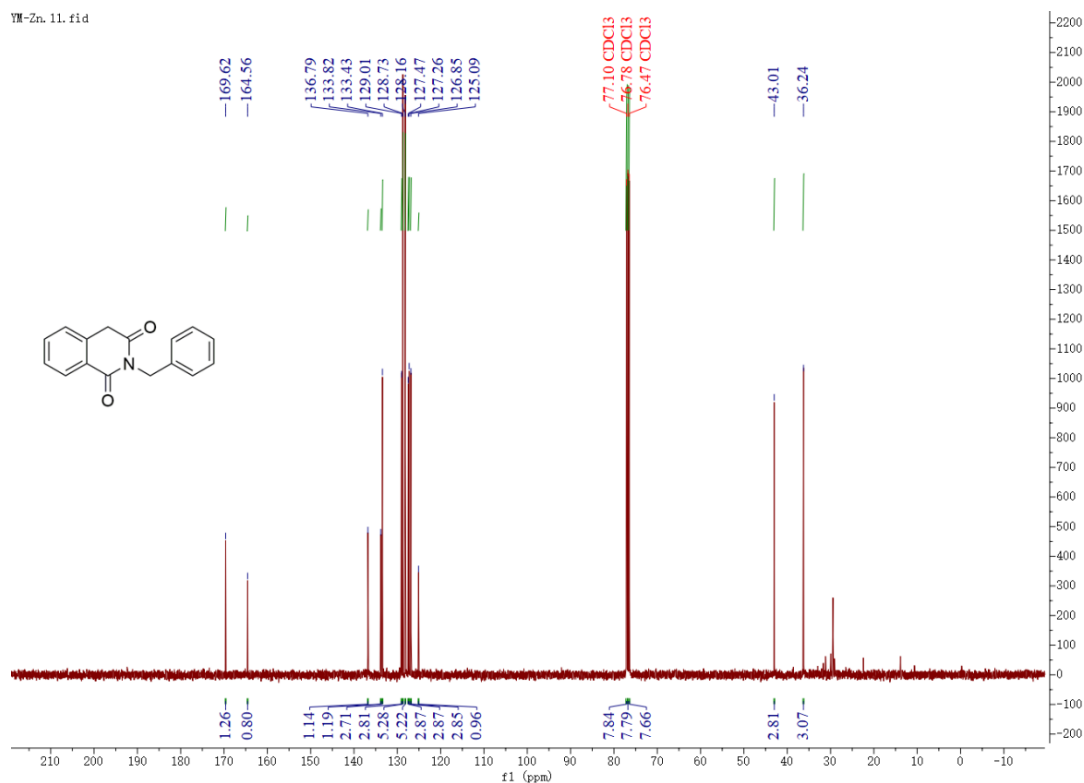




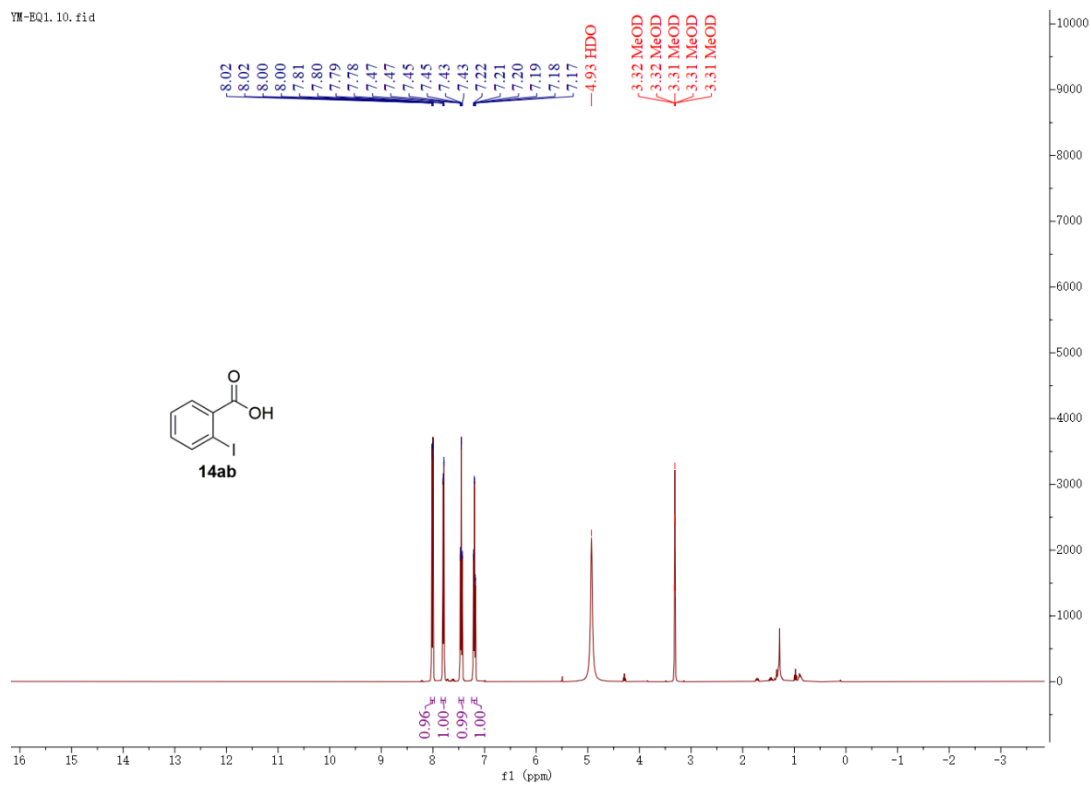
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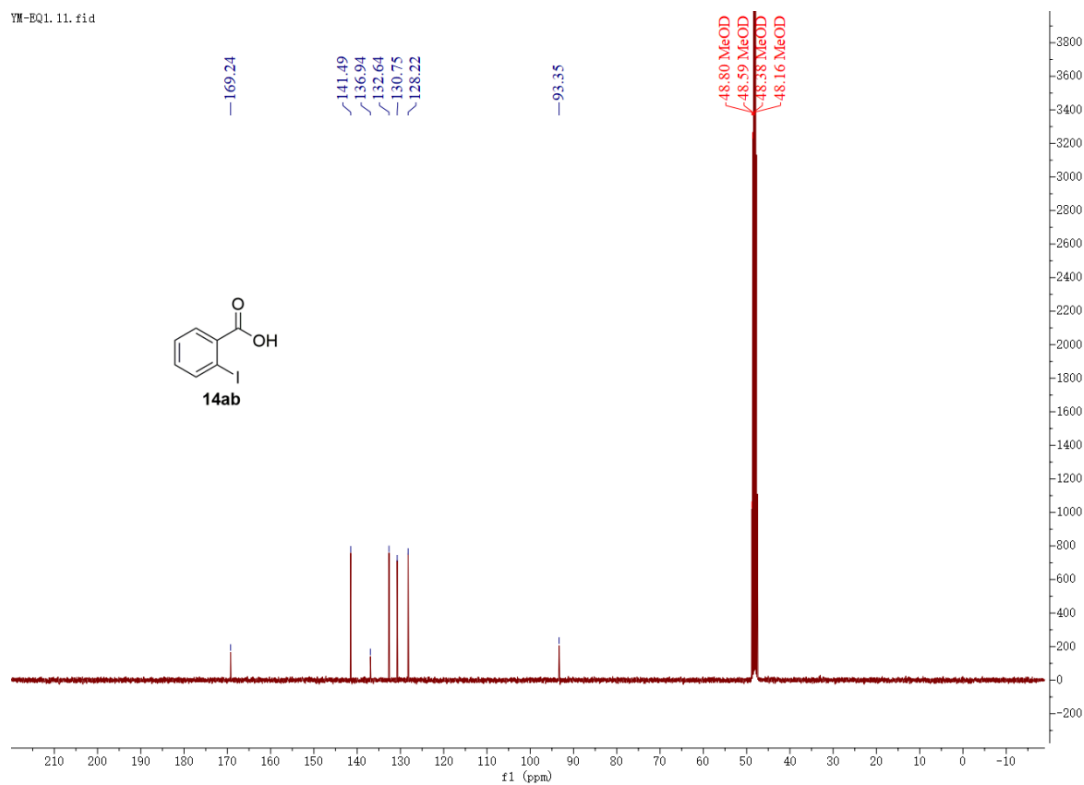
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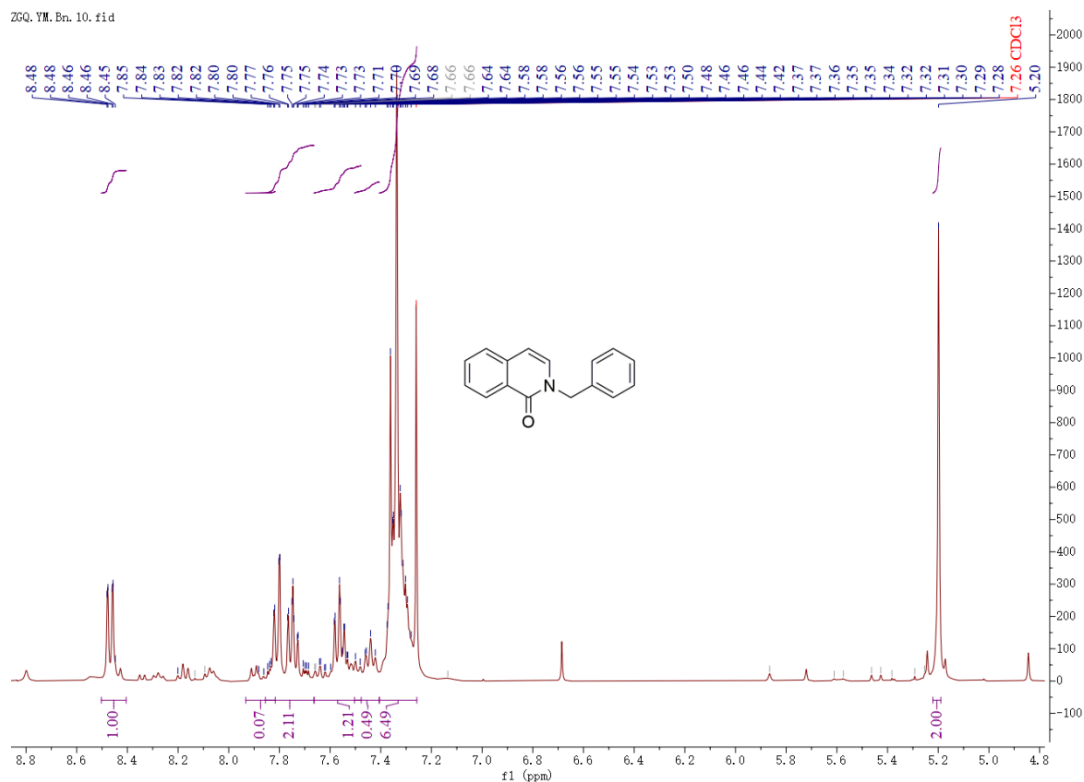
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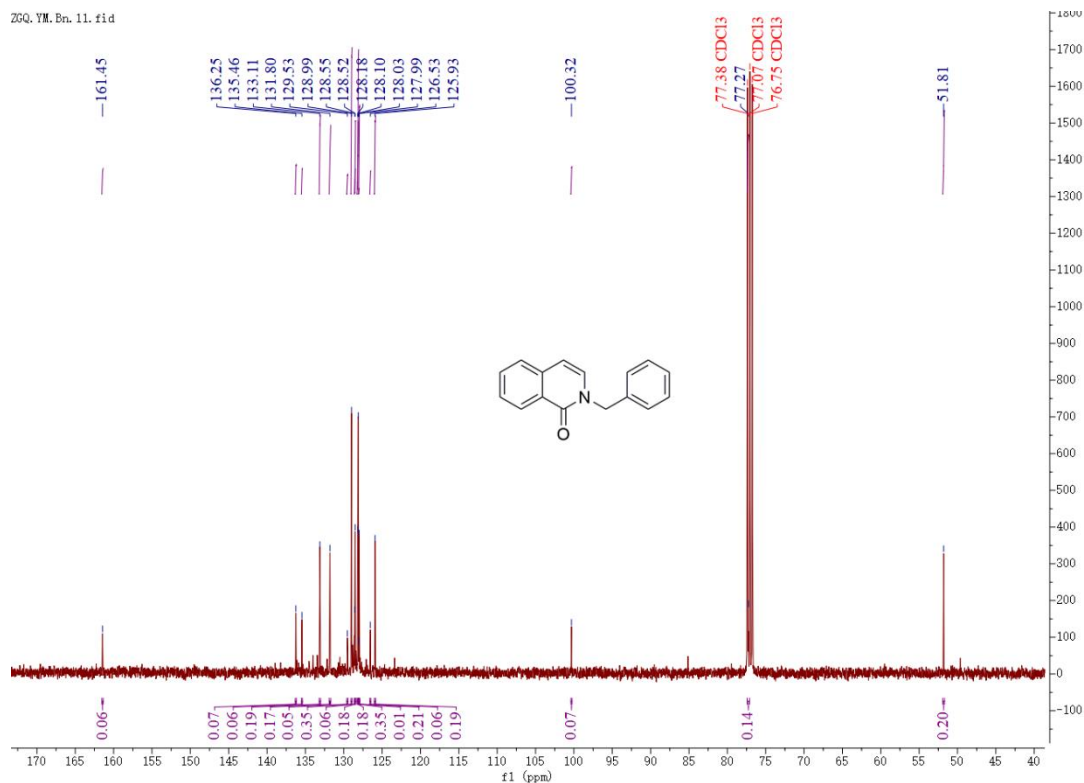
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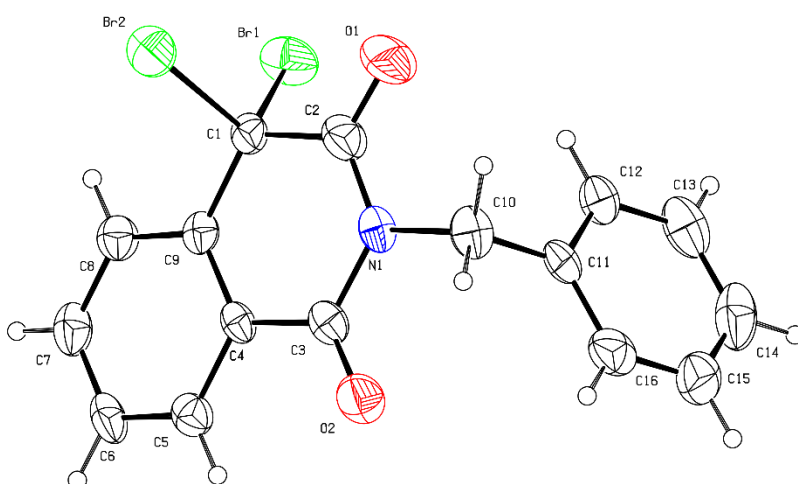
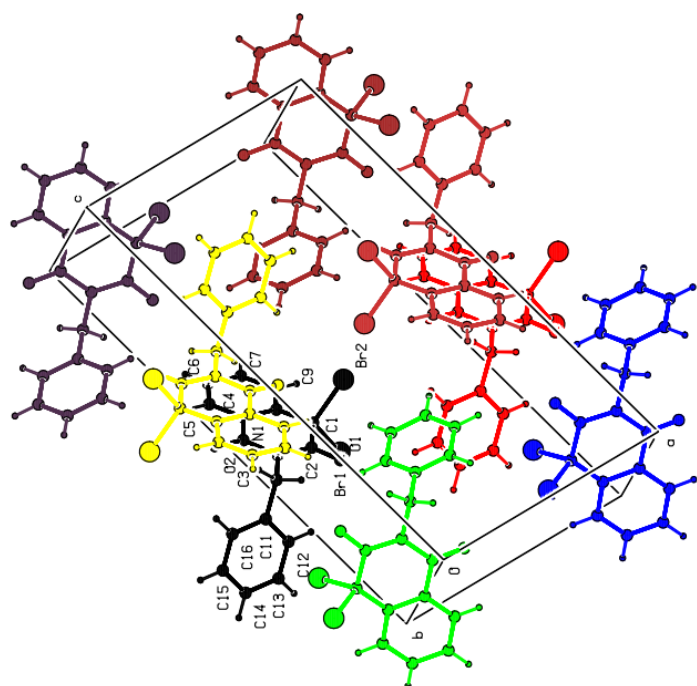


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2. Single crystal structure and data

Single crystal structure of compound 3aa



Compound 3aa single crystal data

Identification code	211027_s2_ycm
Empirical formula	C16H11Br2NO2
Formula weight	409.08
Temperature/K	293.15
Crystal system	monoclinic
Space group	P21/c
a/Å	9.1422 (10)
b/Å	9.3844 (9)
c/Å	17.8359 (18)
α /°	90
β /°	102.960 (10)
γ /°	90
Volume/Å ³	1491.2 (3)
Z	4
ρ calc/cm ³	1.822
μ /mm ⁻¹	5.439
F (000)	800.0
Crystal size/mm ³	0.35 × 0.3 × 0.25
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	6.306 to 52.744
Index ranges	-11 ≤ h ≤ 11, -10 ≤ k ≤ 11, -22 ≤ l ≤ 21
Reflections collected	6451
Independent reflections	3054 [Rint = 0.0481, Rsigma = 0.1031]
Data/restraints/parameters	3054/0/190
Goodness-of-fit on F ²	0.967
Final R indexes [$I \geq 2\sigma(I)$]	R1 = 0.0553, wR2 = 0.0966
Final R indexes [all data]	R1 = 0.1401, wR2 = 0.1241
Largest diff. peak/hole / e Å ⁻³	0.41/-0.58
