Supporting Information

Development of novel amino-quinoline-5,8-dione derivatives as NAD(P)H: quinone oxidoreductase 1 (NQO1) inhibitors with potent antiproliferative activities

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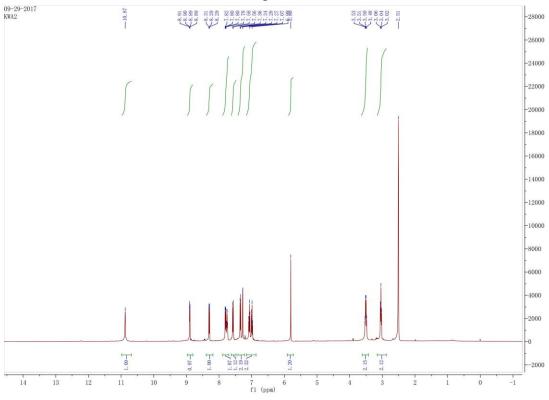
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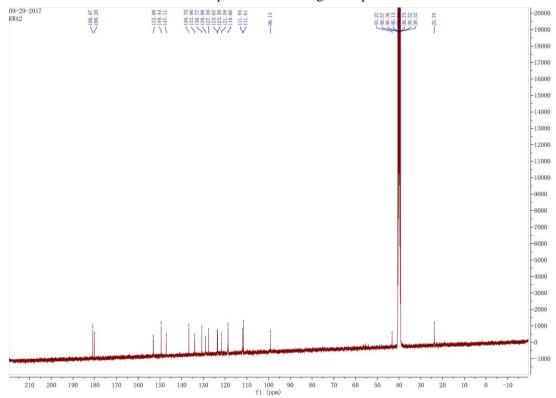
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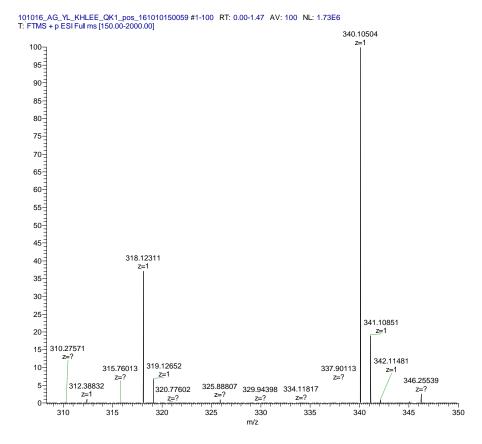
1.The ¹H NMR, ¹³C NMR, and HRMS spectra for **6a-h** and **7a-h**



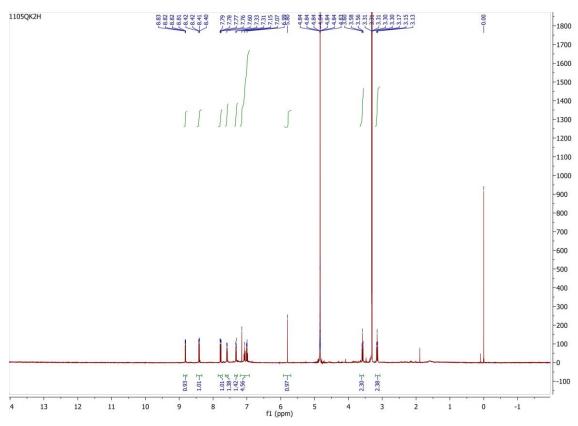
¹H NMR spectrum of the target compound **6a**



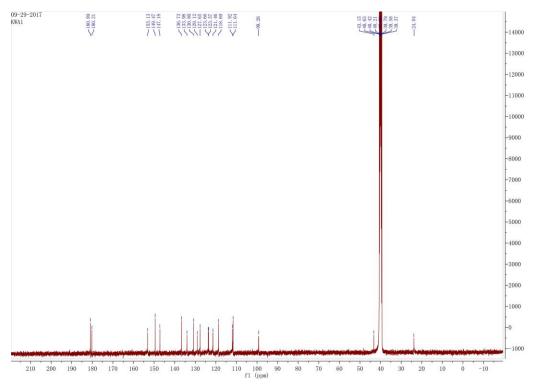
¹³C NMR spectrum of the target compound **6a**



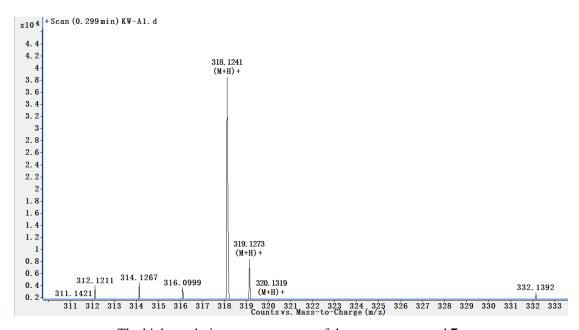
The high resolution mass spectrum of the target compound 6a



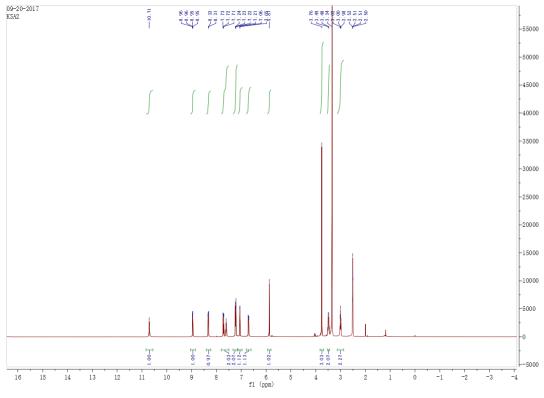
¹H NMR spectrum of the target compound **7a**



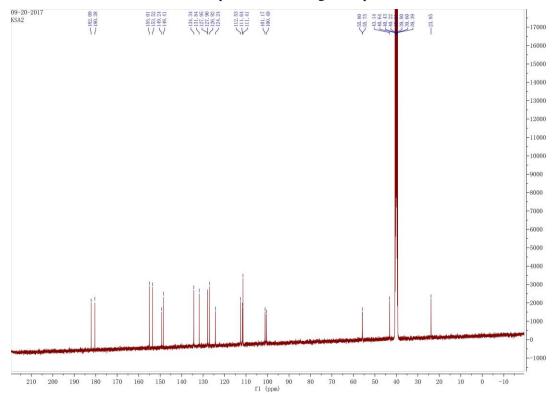
¹³C NMR spectrum of the target compound **7a**



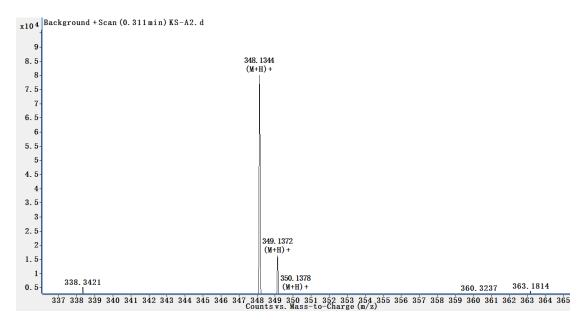
The high resolution mass spectrum of the target compound 7a



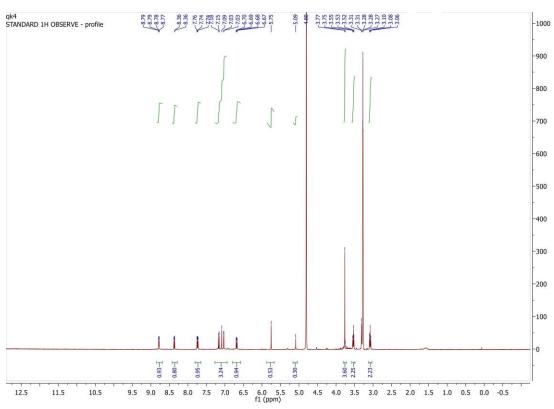
¹H NMR spectrum of the target compound **6b**



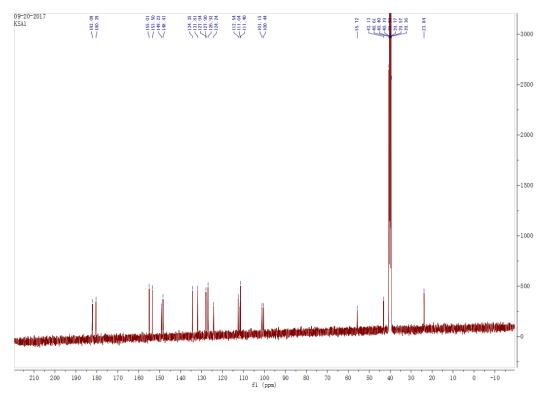
¹³C NMR spectrum of the target compound **6b**



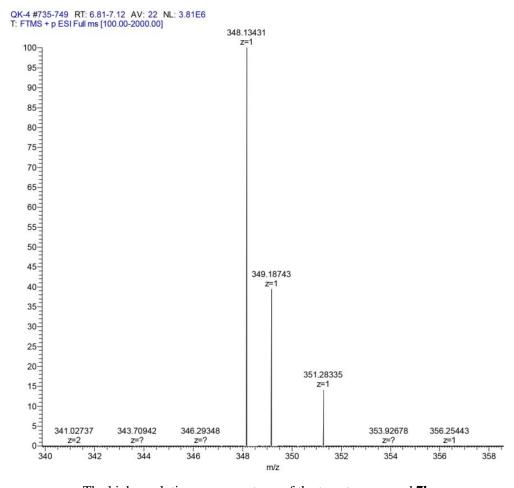
The high resolution mass spectrum of the target compound ${\bf 6b}$



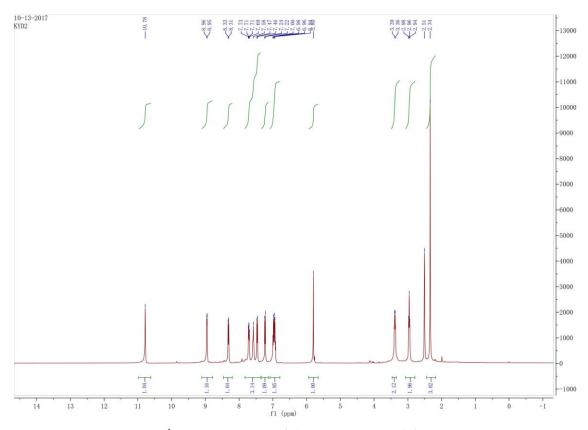
¹H NMR spectrum of the target compound **7b**



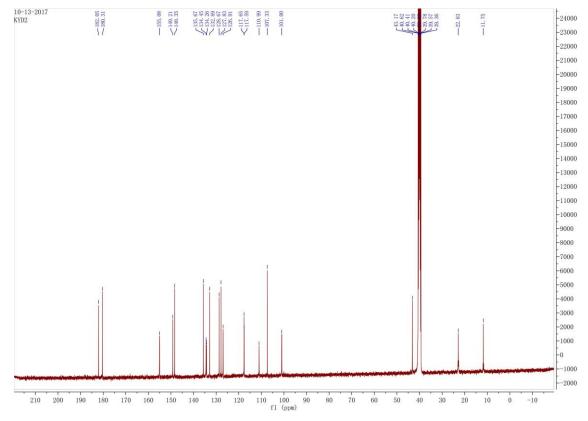
¹³C NMR spectrum of the target compound **7b**



The high resolution mass spectrum of the target compound 7b

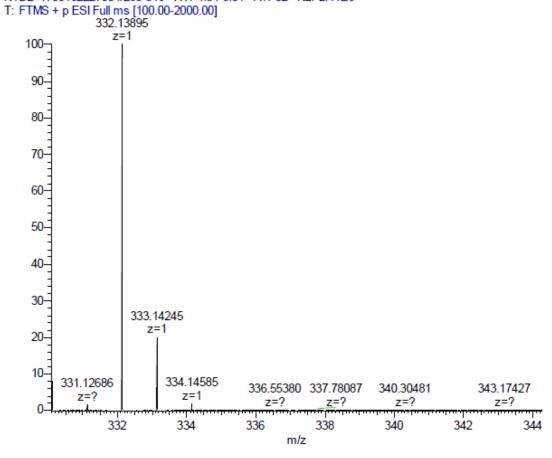


¹H NMR spectrum of the target compound **6c**

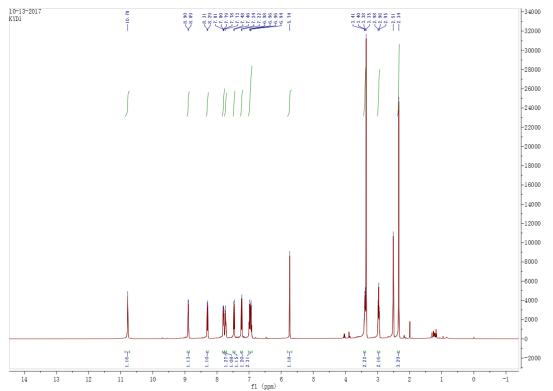


¹³C NMR spectrum of the target compound **6c**

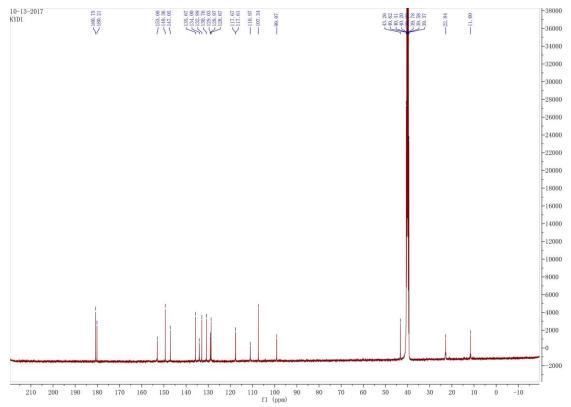
KYD2 170516222700 #285-316 RT: 4.54-5.01 AV: 32 NL: 2.41E6



The high resolution mass spectrum of the target compound $\mathbf{6c}$

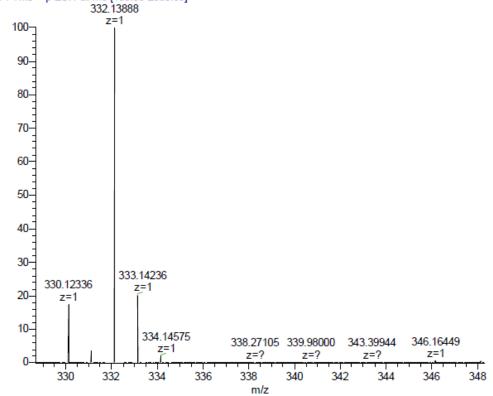


 ^{1}H NMR spectrum of the target compound 7c

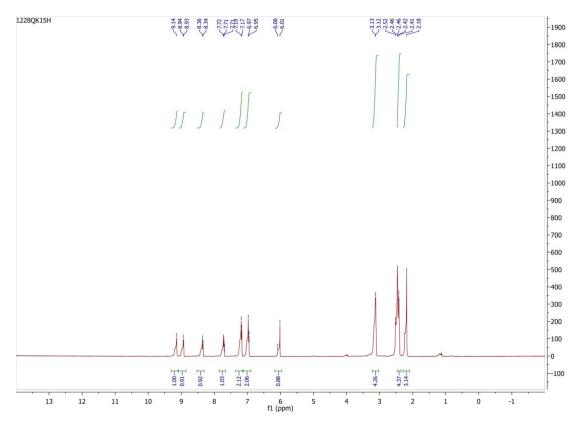


¹³C NMR spectrum of the target compound **7c**

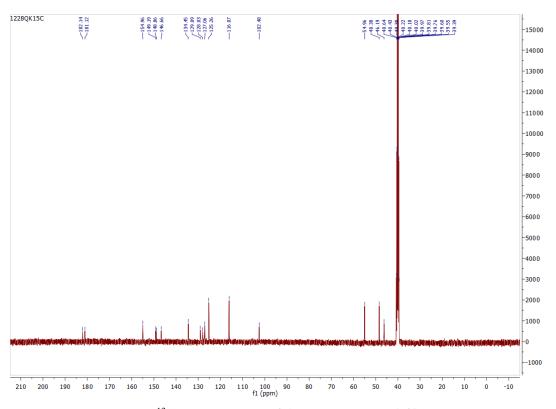




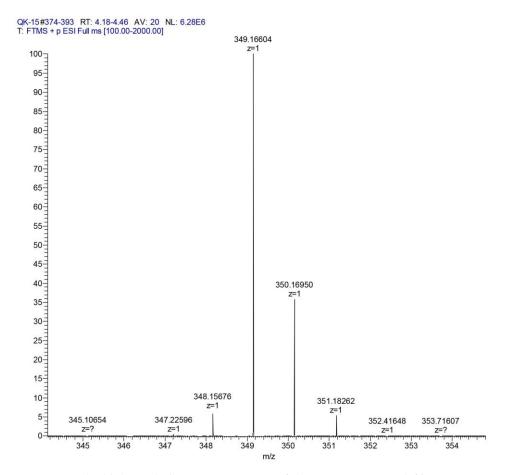
The high resolution mass spectrum of the target compound 7c



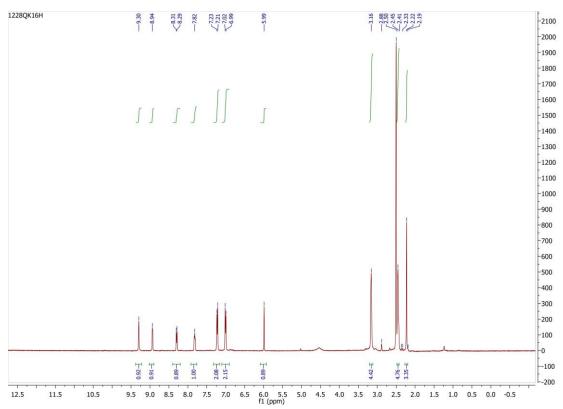
¹H NMR spectrum of the target compound **6d**



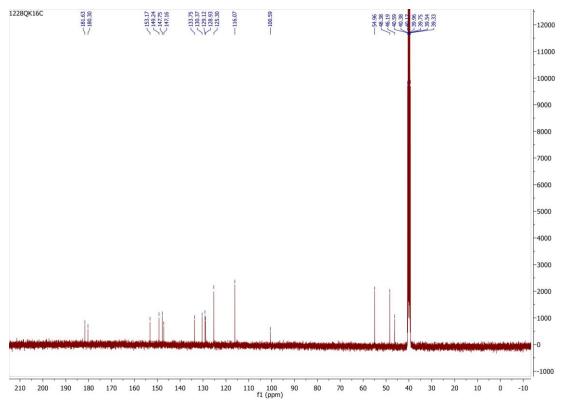
¹³C NMR spectrum of the target compound **6d**



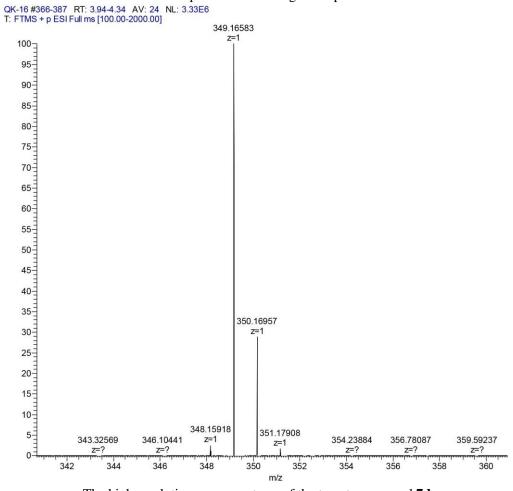
The high resolution mass spectrum of the target compound 6d



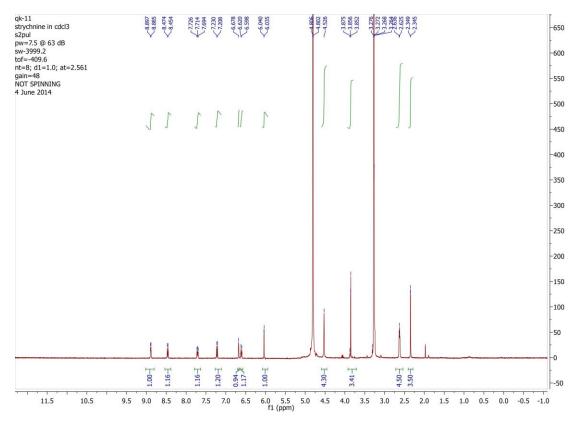
¹H NMR spectrum of the target compound **7d**



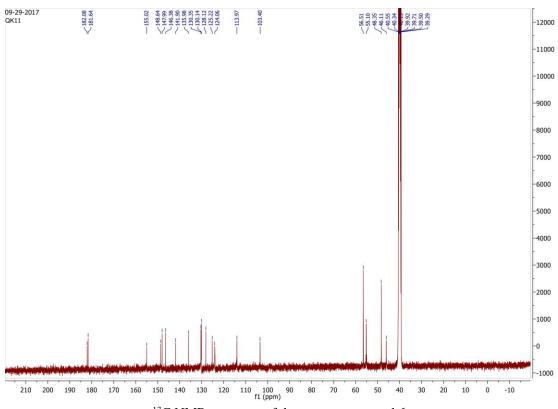
¹³C NMR spectrum of the target compound **7d**



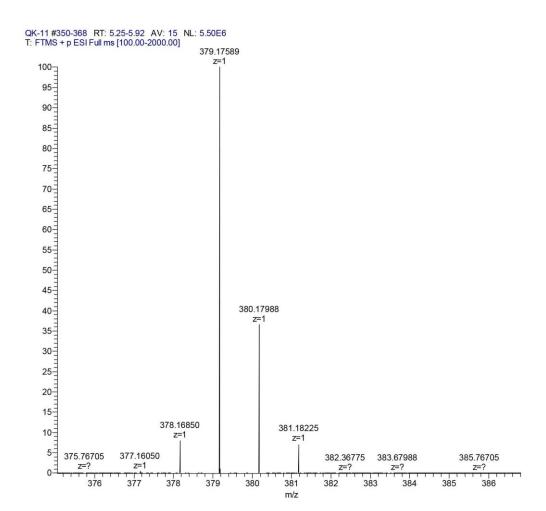
The high resolution mass spectrum of the target compound $\mathbf{7d}$

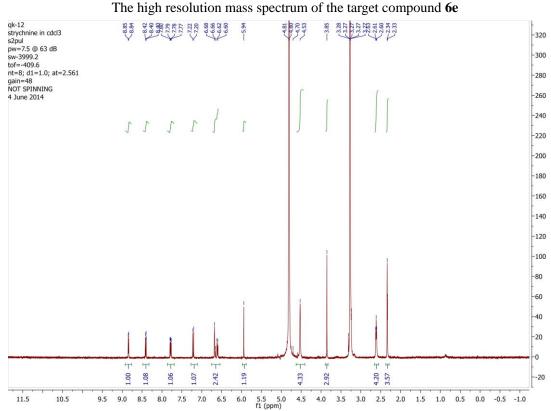


¹H NMR spectrum of the target compound **6e**

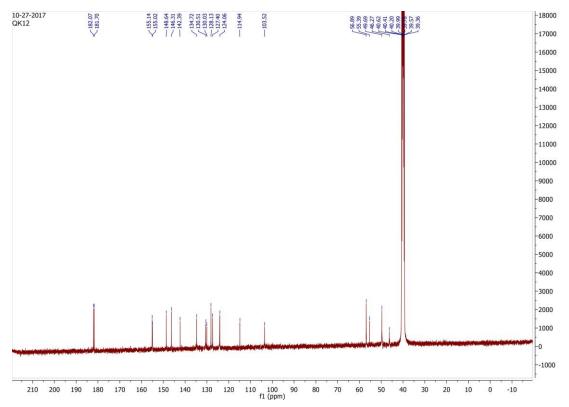


¹³C NMR spectrum of the target compound **6e**

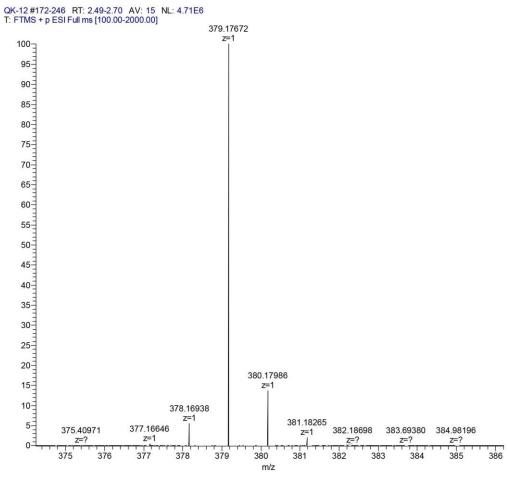




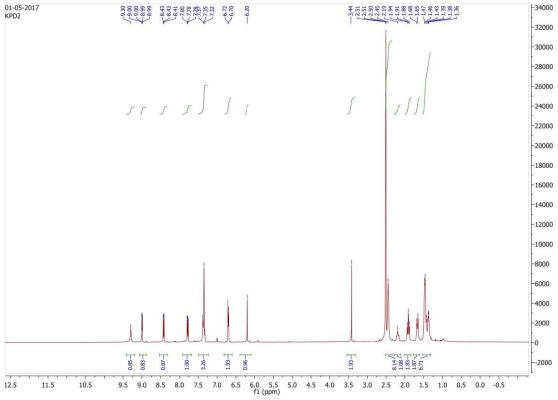
 ^{1}H NMR spectrum of the target compound 7e



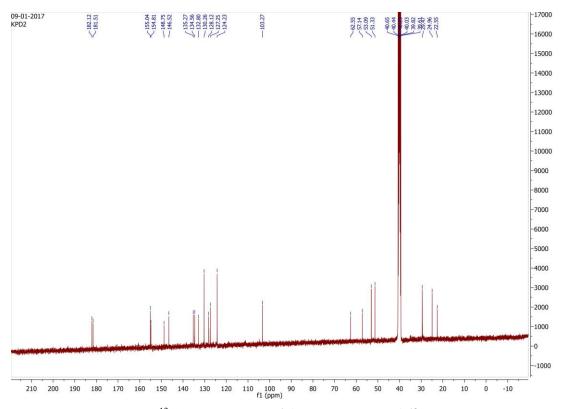
¹³C NMR spectrum of the target compound **7e**



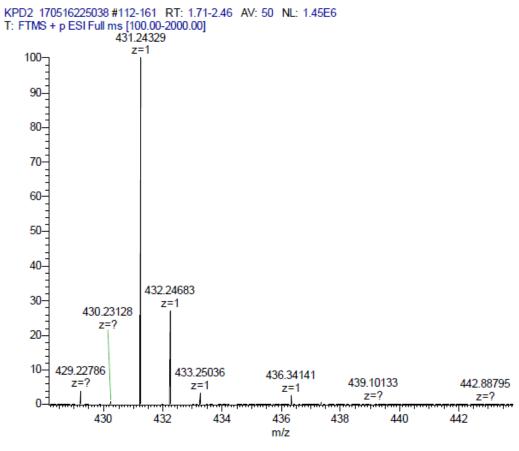
The high resolution mass spectrum of the target compound 7e



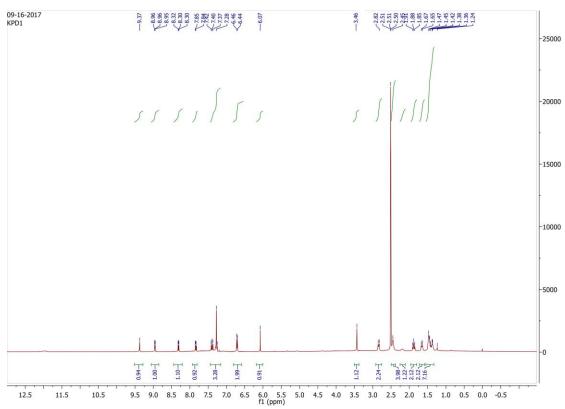
¹H NMR spectrum of the target compound 6f



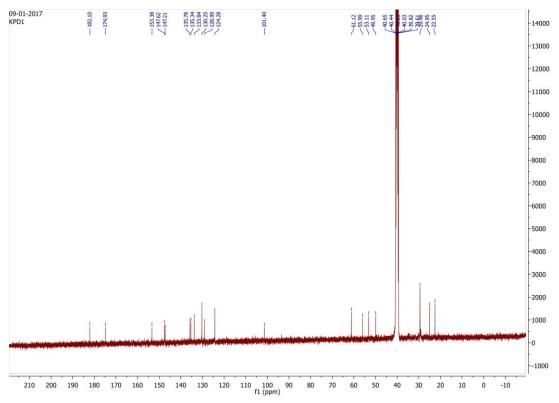
¹³C NMR spectrum of the target compound **6f**



The high resolution mass spectrum of the target compound 6f

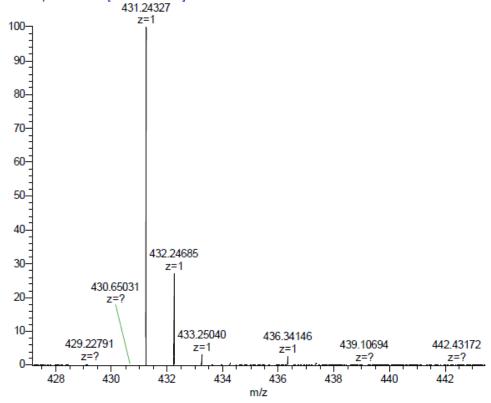


¹H NMR spectrum of the target compound **7f**

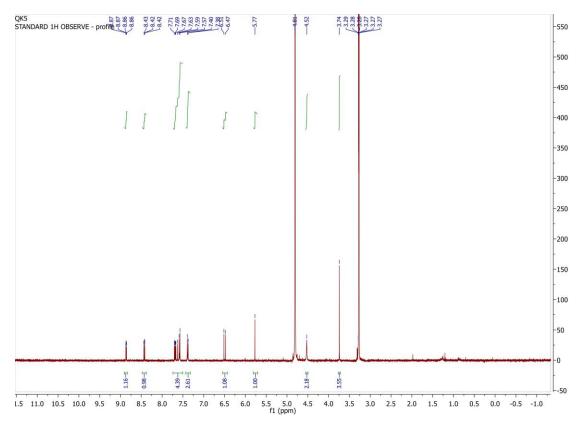


¹³C NMR spectrum of the target compound **7f**

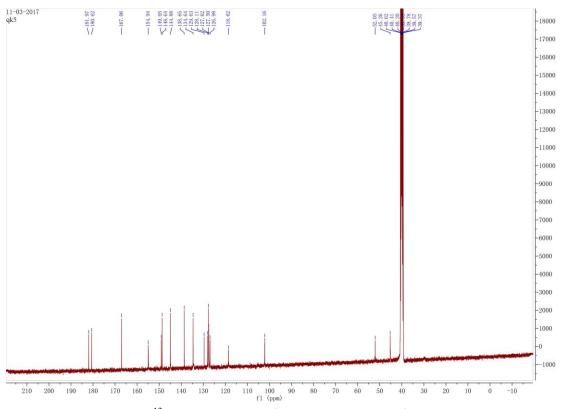




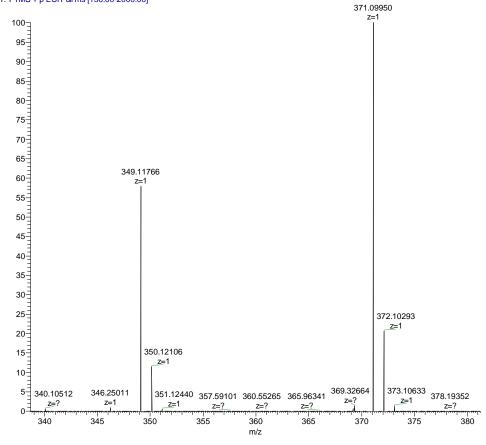
The high resolution mass spectrum of the target compound 7f



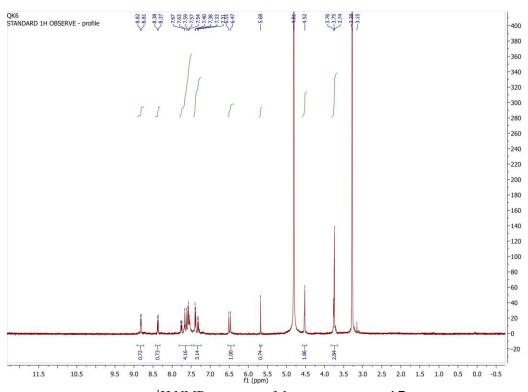
 ^{1}H NMR spectrum of the target compound $\mathbf{6g}$



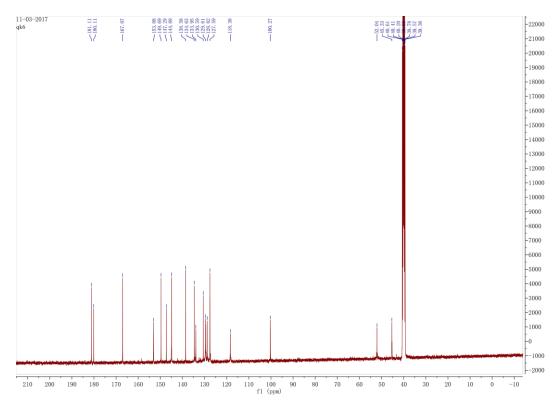
¹³C NMR spectrum of the target compound **6g**



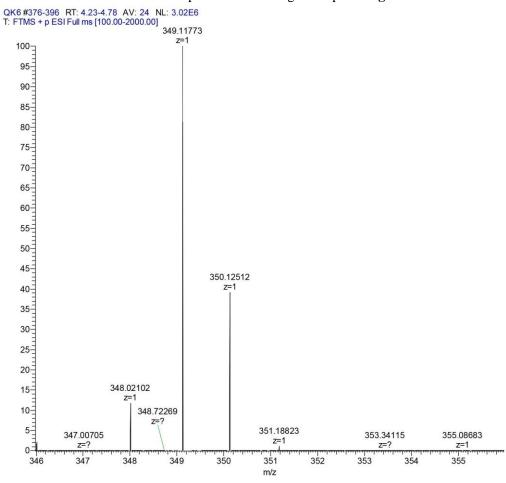
The high resolution mass spectrum of the target compound $\mathbf{6g}$



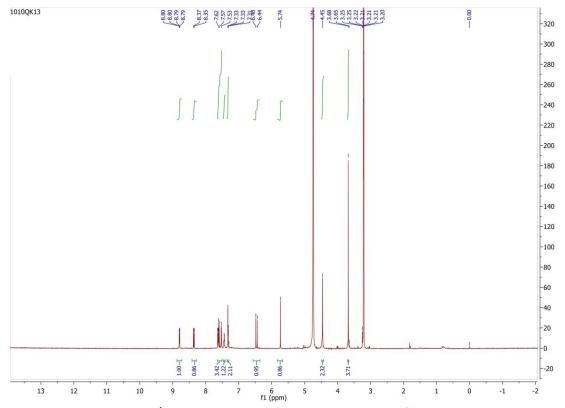
¹H NMR spectrum of the target compound **7g**



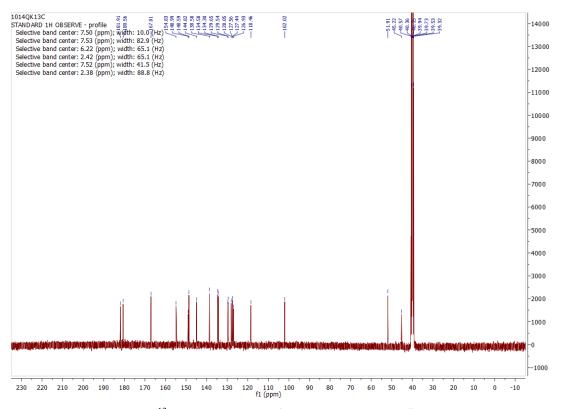
¹³C NMR spectrum of the target compound **7g**



The high resolution mass spectrum of the target compound 7g



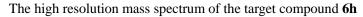
¹H NMR spectrum of the target compound **6h**

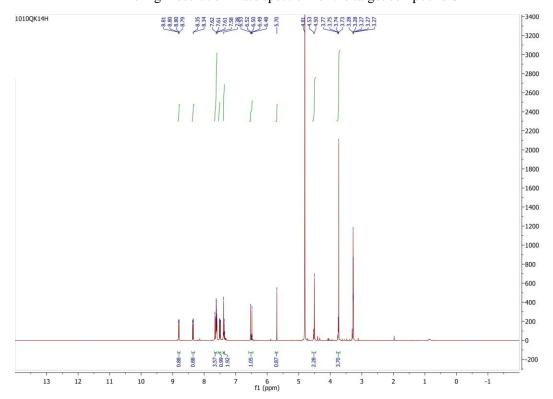


¹³C NMR spectrum of the target compound **6h**

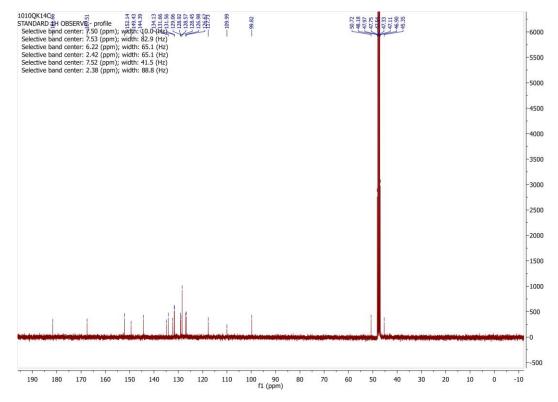


45= 350.12490 40= 35 30= 25 20-15-10-351.14946 5 348.74965 354.22800 352.55565 353.24271 0-349 348 350 351 352 m/z

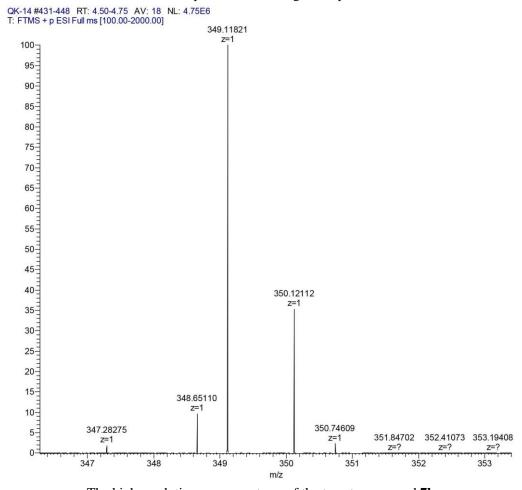




¹H NMR spectrum of the target compound **7h**



¹³C NMR spectrum of the target compound **7h**



The high resolution mass spectrum of the target compound $\mathbf{7h}$

2. HPLC assessment of compound purity.

Target compound **6a-h** and **7a-h** with a purity of >95% (HPLC analysis) were used for subsequent experiments. We provided the spectra of HPLC assays as below.

Column: Inertex C18 (150mm×4.6mm×5µm);

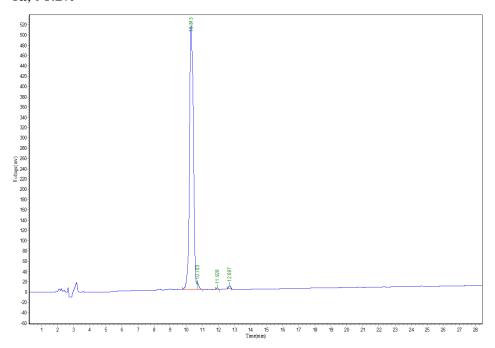
Mobile phase: Methanol: ammonium acetate buffer (32 mmol/L, pH 5.0) = $75:25 \sim$

90:10;

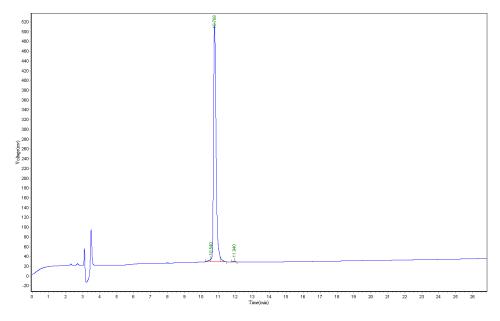
Wavelength: 254 nm;

Rate: 1 ml/min; Temperature: 30 ℃; Pressure: 89-122 kgf.

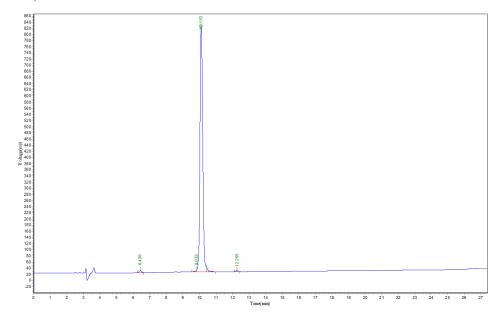
6a, 98.2%



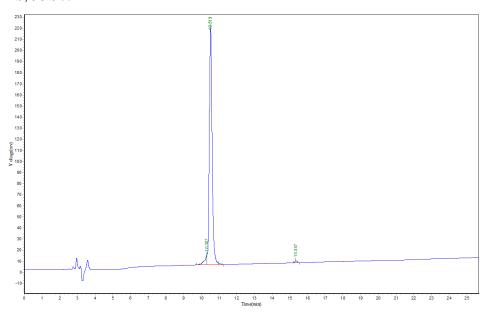
7a, 98.2%



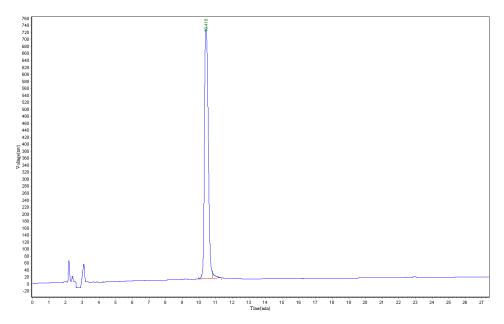
6b, 97.5%



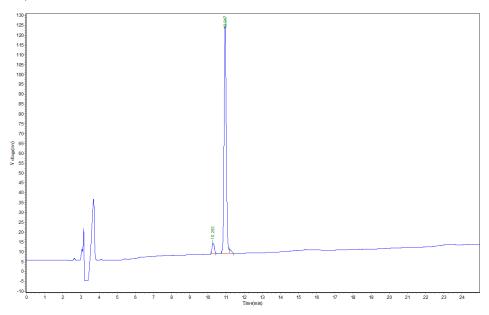
7b, 95.9%



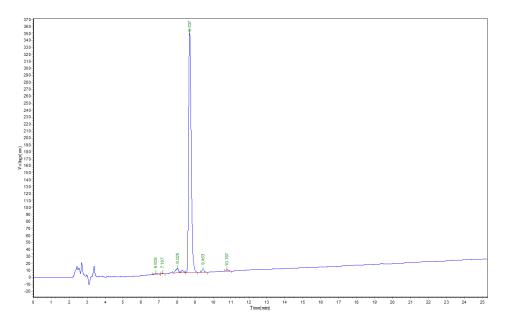
6c, 98.5%



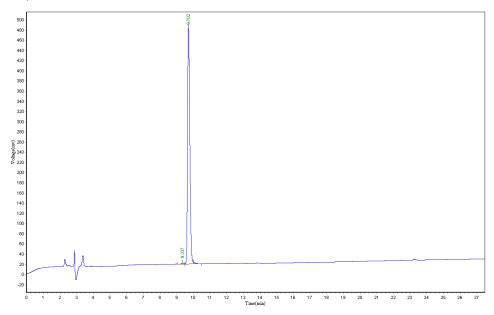
7c, 95.2%



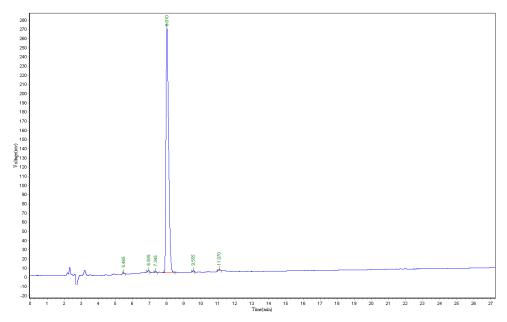
6d, 95.4%



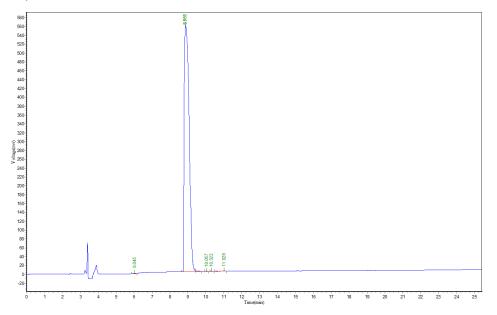
7d, 98.8%



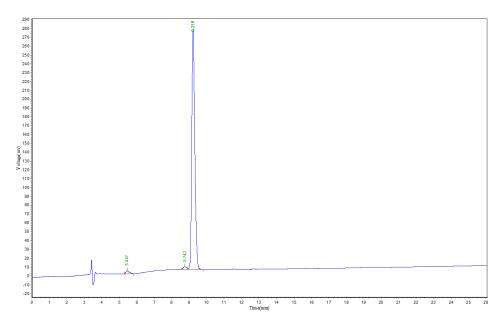
6e, 98.4%



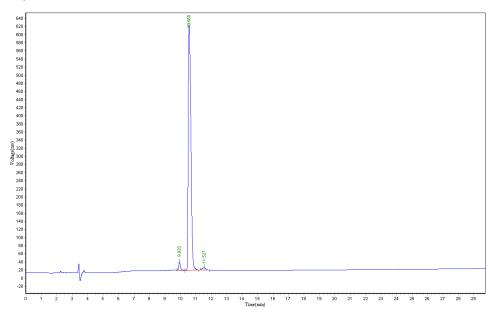
7e, 99.6%



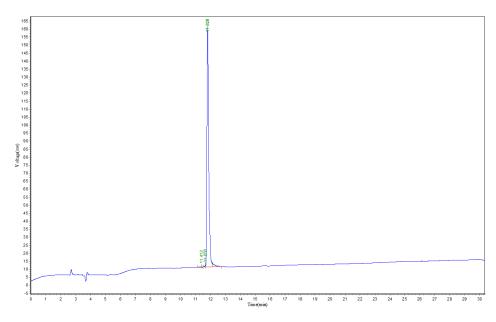
6f, 97.3%



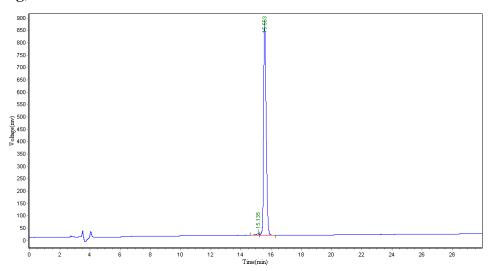
7f, 96.8%



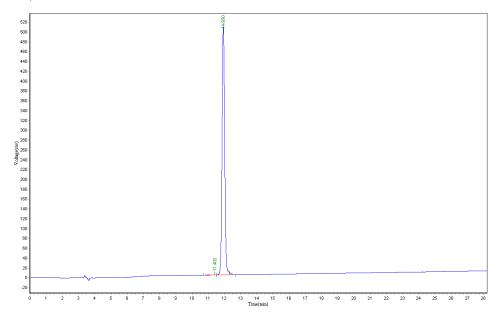
6g, 98.0%



7g, 99.0%



6h, 99.3%



7h, 95.4%

