Supporting information for

$AlCl_3 \cdot 6H_2O$-Catalyzed Friedel–Crafts Alkylation of Indoles by *para*-Quinone Methide moiety of Celastrol

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Contents

1. Regioselectivity analysis of our reaction

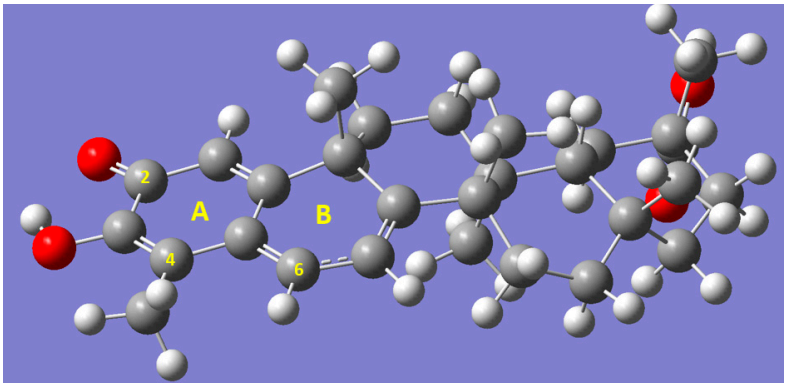
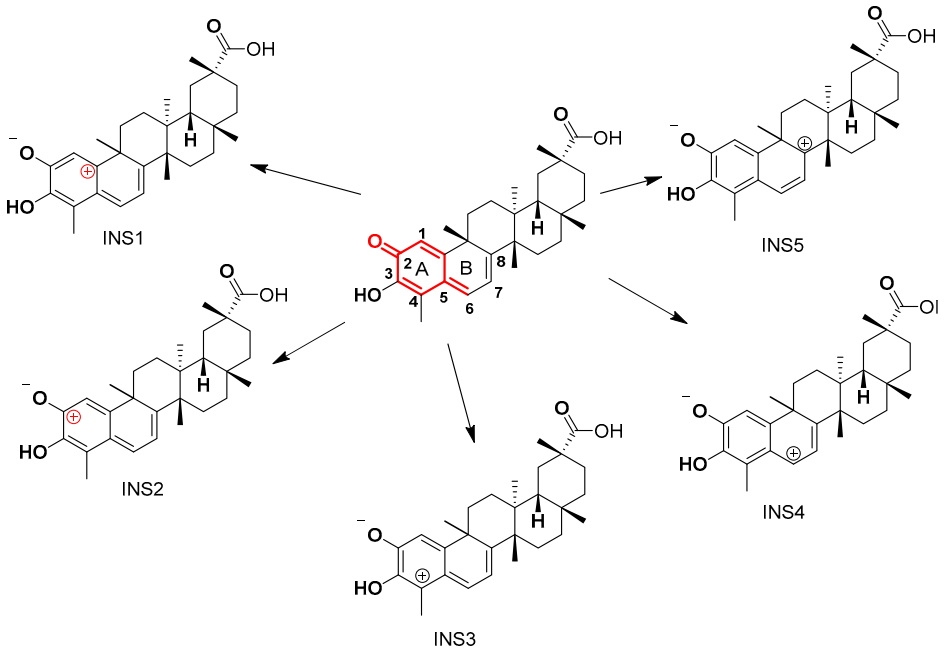
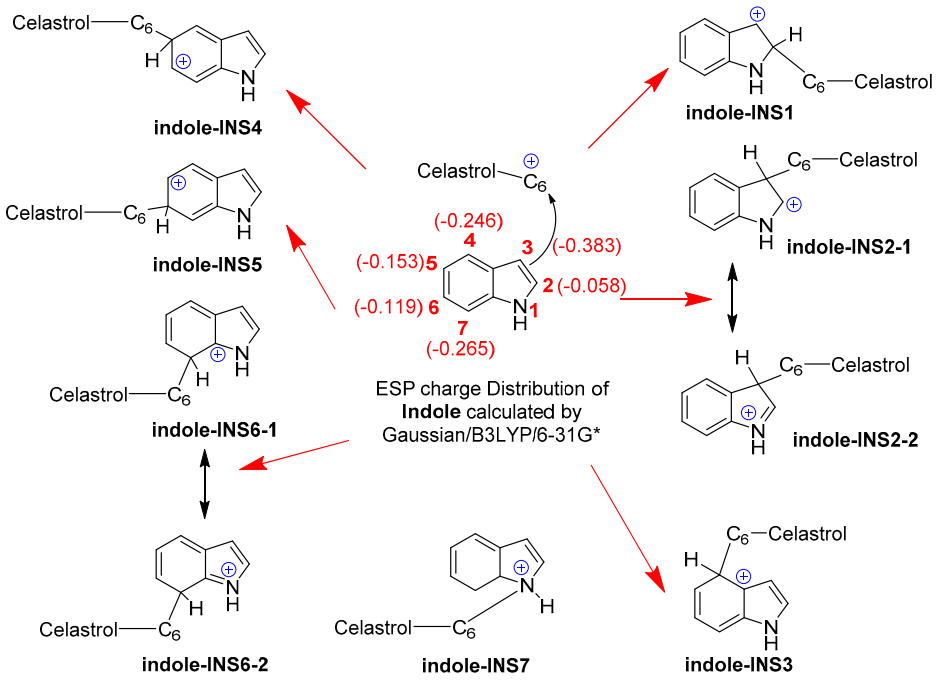


Figure S1. The 3D structure of celastrol



Scheme S1. The possible carbocationic intermediates produced by celastrol



Scheme S2. The possible intermediates produced by indole

2. HPLC method for the determination of reaction yield in screening

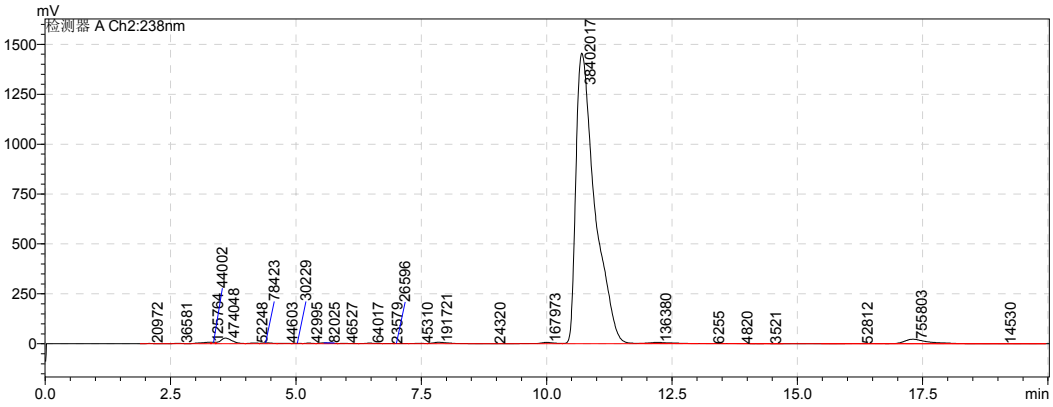


Figure S2. The HPLC spectrum of 2 mg/mL **3a**

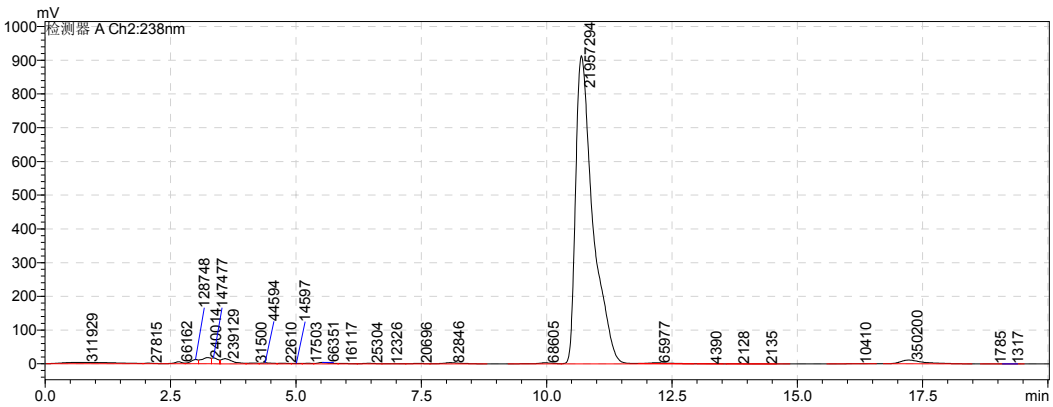


Figure S3. The HPLC spectrum of 1 mg/mL 3a

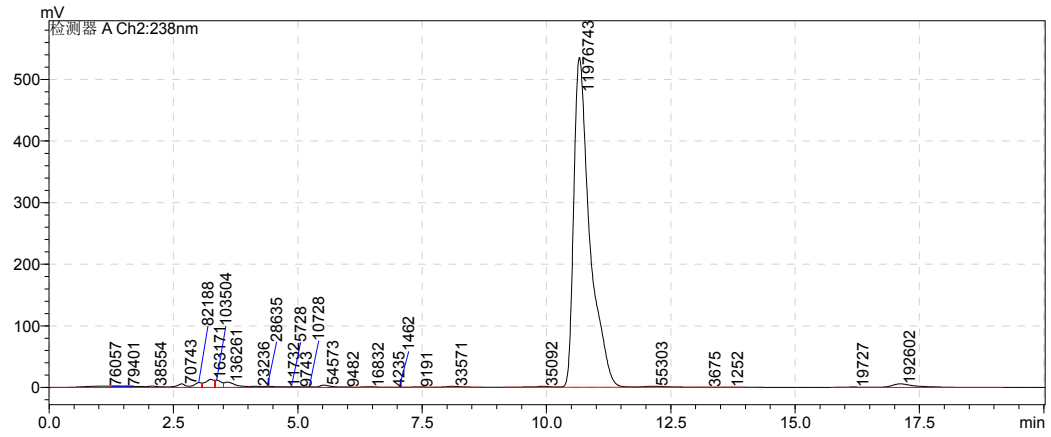


Figure S4. The HPLC spectrum of 0.5 mg/mL 3a

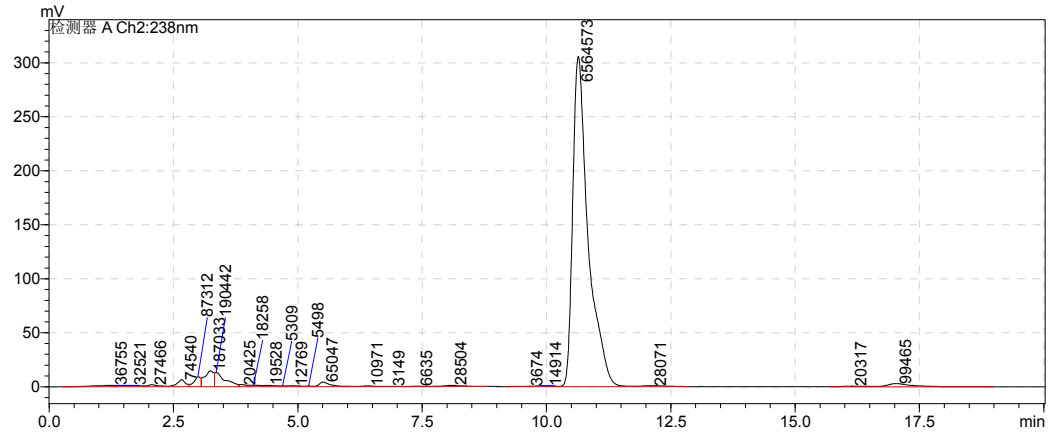


Figure S5. The HPLC spectrum of 0.25 mg/mL 3a

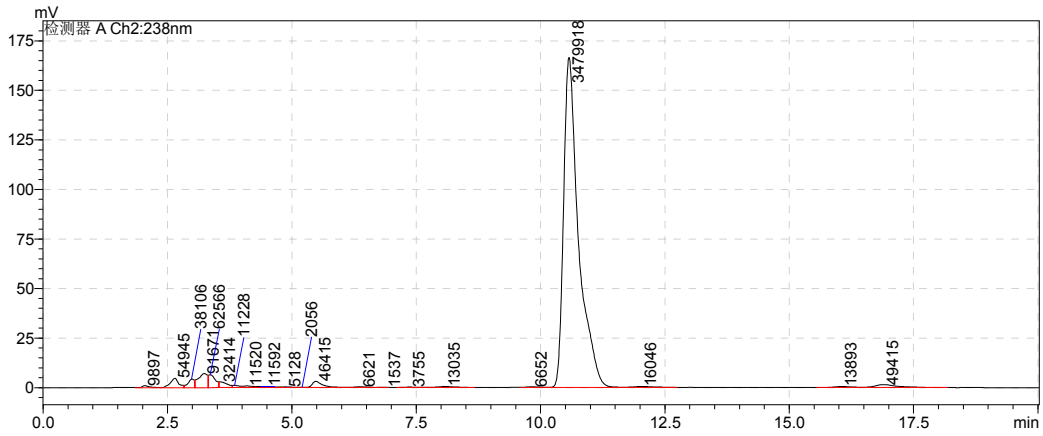


Figure S6. The HPLC spectrum of 0.125 mg/mL 3a

Table S1. The summarized HPLC results of **3a** with different concentrations

Entry	Retention (min)	Concentration (mg/mL)	Peak area
1	10.698	2	38402017
2	10.690	1	21957294
3	10.657	0.5	11976743
4	10.634	0.25	6564573
5	10.568	0.125	3479918

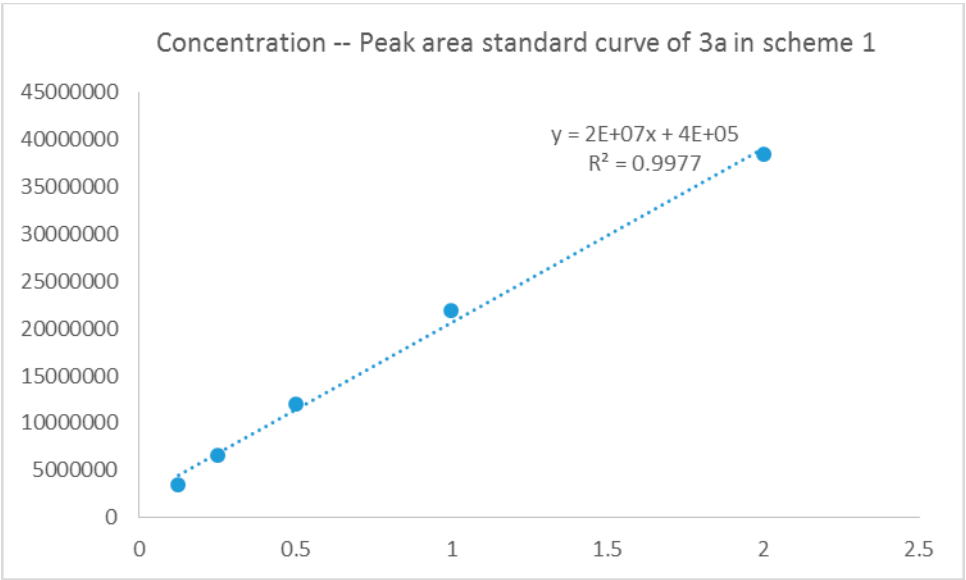


Figure S7. Concentration – Peak area standard curve of 3a

Fitting formula:

$y = 2E+07x + 4E+05$ $R^2 = 0.9977$

3. HPLC spectra and results of reaction optimization in Table 1

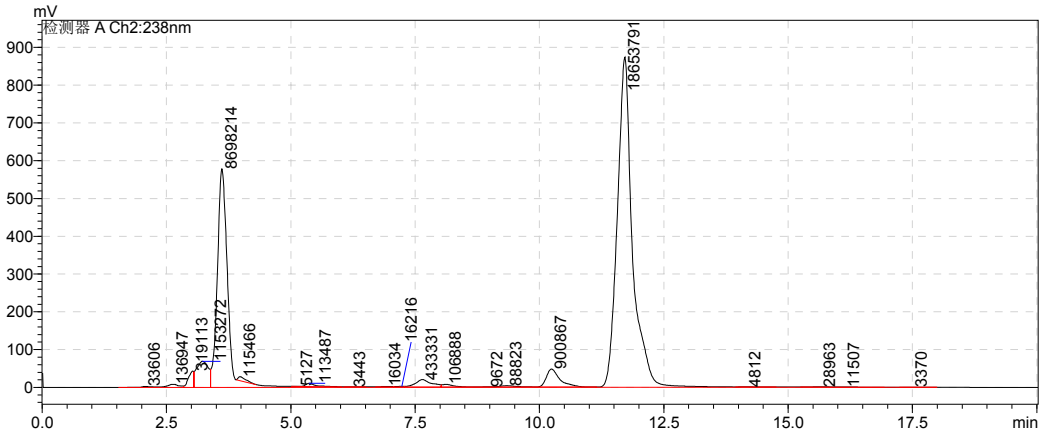


Figure S8 The HPLC spectrum of entry 1 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.238	900867	0.6	**2 %**
1a	11.711	18653791		

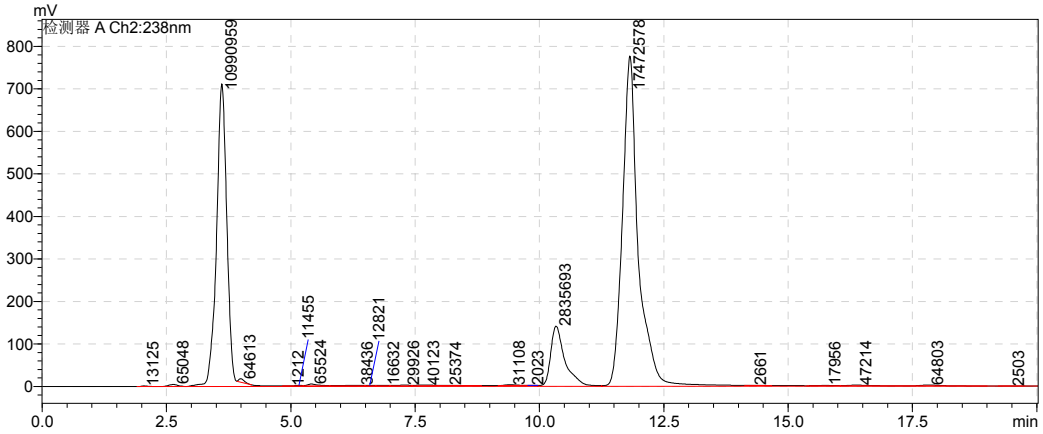


Figure S9 The HPLC spectrum of entry 2 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.329	2835693	3.0	**12 %**
1a	11.815	17472578		

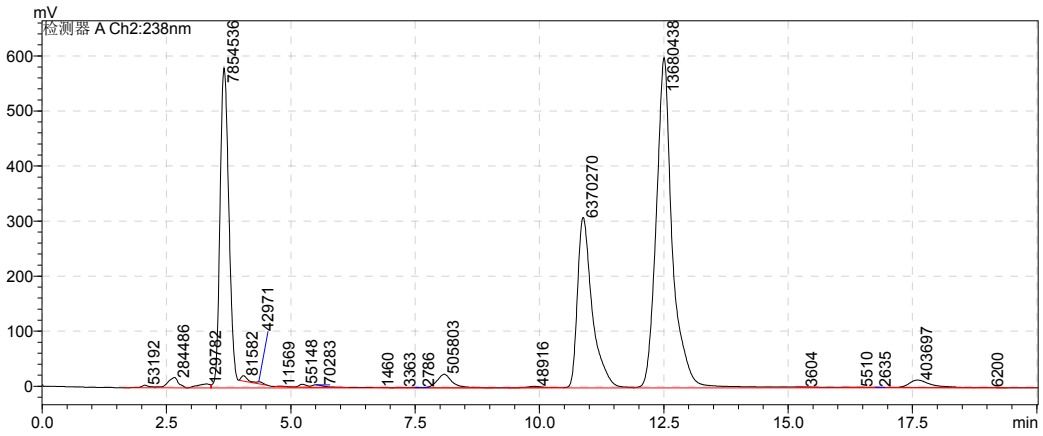


Figure S10 The HPLC spectrum of entry 3 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.873	6370270	7.5	**28 %**
1a	12.501	13680438		

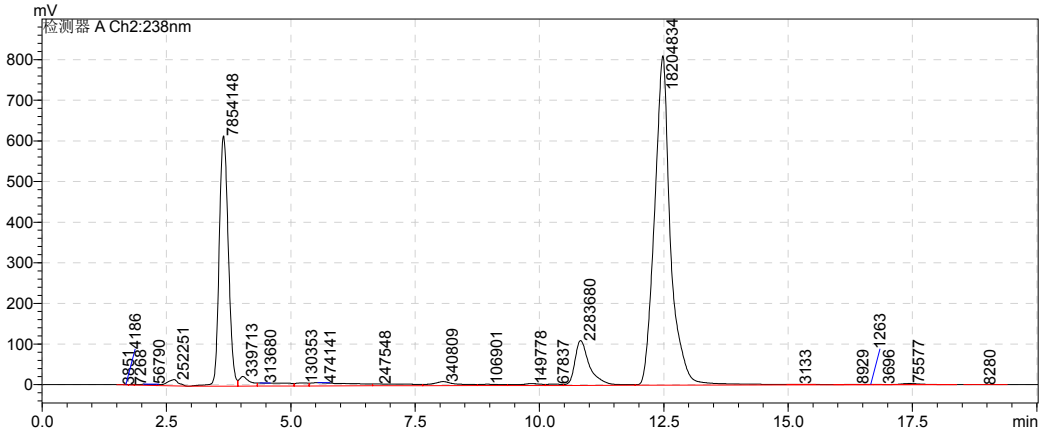


Figure S11 The HPLC spectrum of entry 4 in table 1

compound	Retention time	Peak area	Amount of (mg)	Yield
2a	1	2283680	2.3	**9 %**
1a	2	18204834		

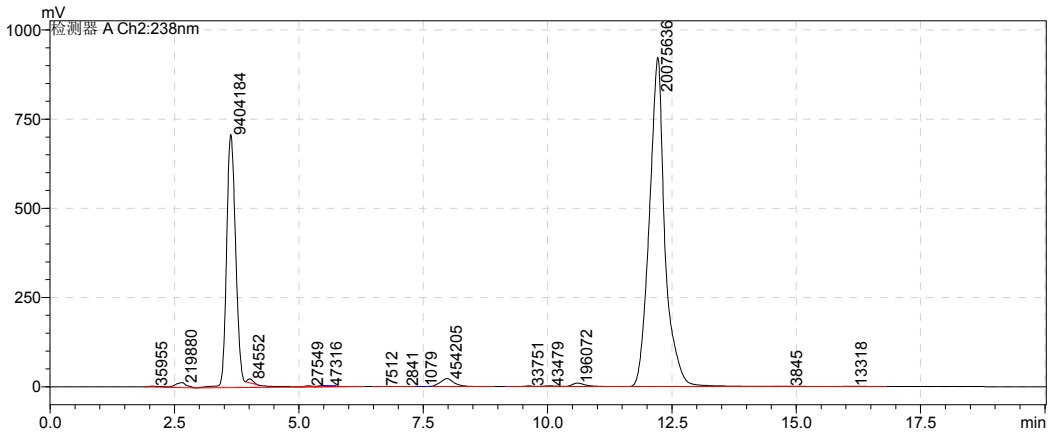


Figure S12 The HPLC spectrum of entry 5 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.599	196072	0	**0 %**
1a	12.212	20075636		

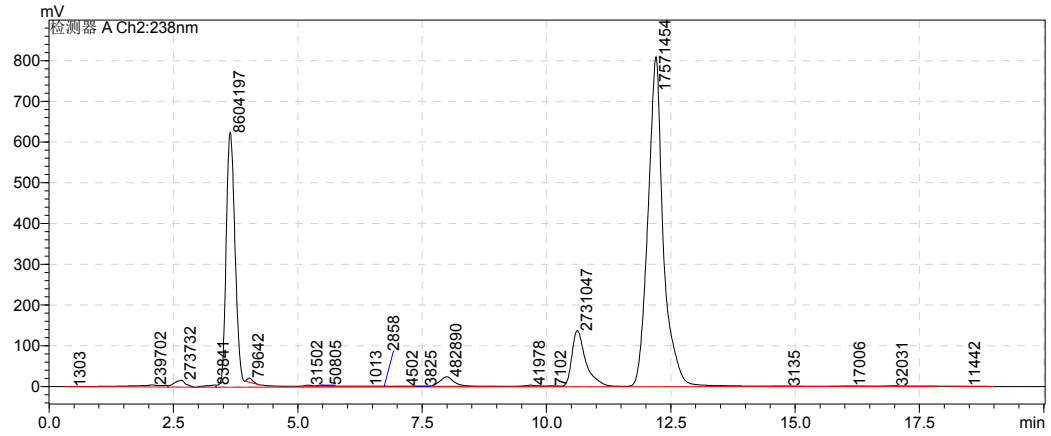


Figure S13 The HPLC spectrum of entry 6 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.615	2731047	2.9	**11 %**
1a	12.197	17571454		

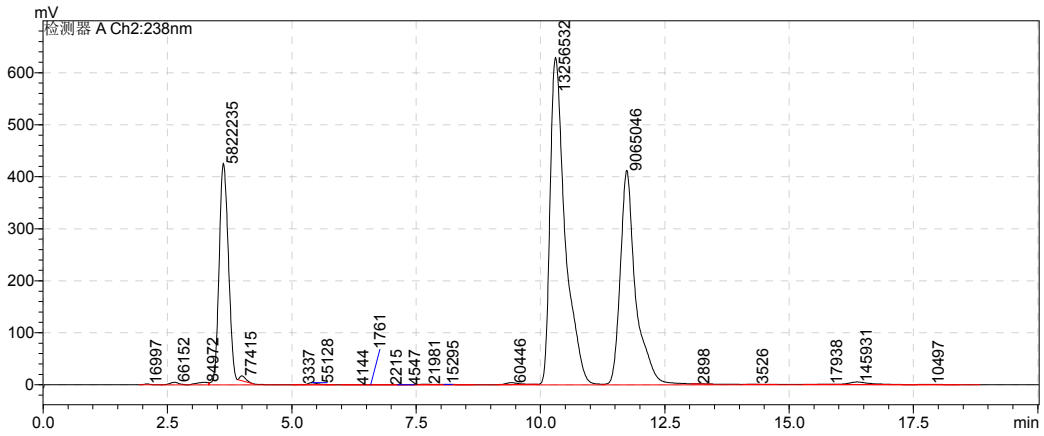


Figure S14 The HPLC spectrum of entry 7 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.298	13256532	16.1	**64 %**
1a	11.731	9065046		

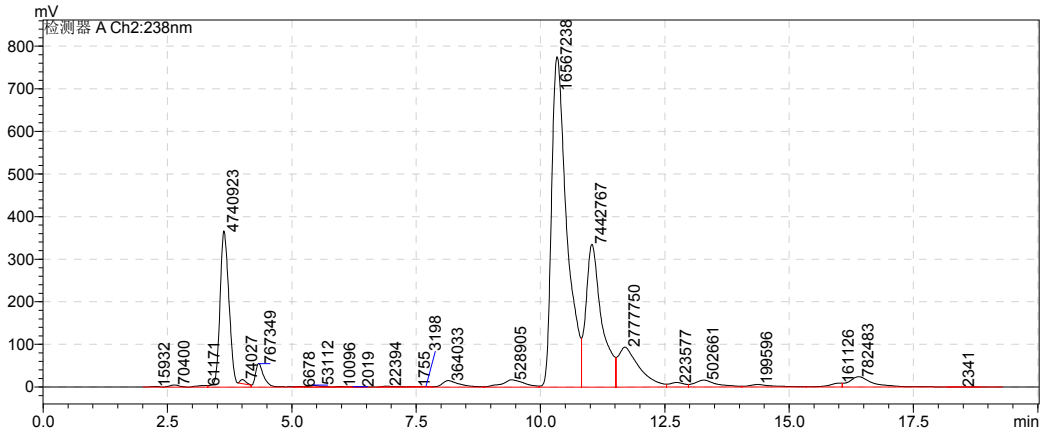


Figure S15 The HPLC spectrum of entry 8 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.330	16567238	20.2	**80 %**
1a	11.694	2777750		

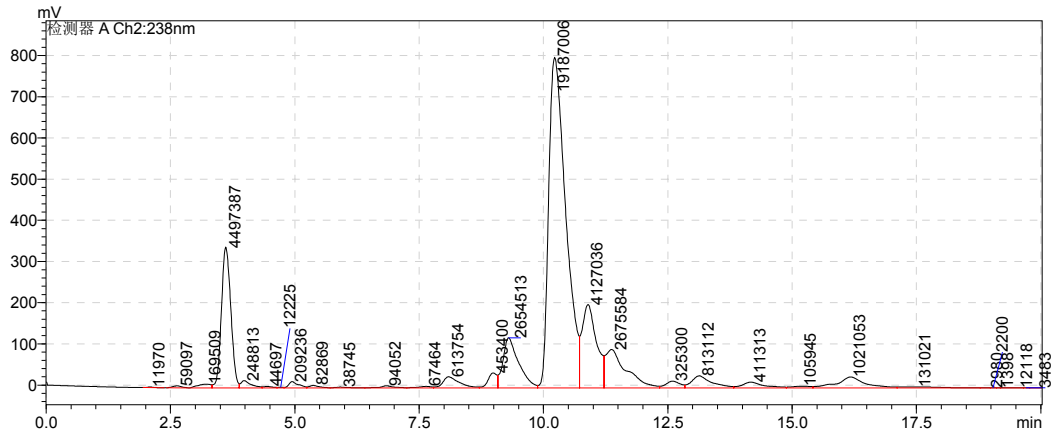


Figure S16 The HPLC spectrum of entry 9 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.220	19187006	23.5	**93 %**
1a	11.365	2675584		

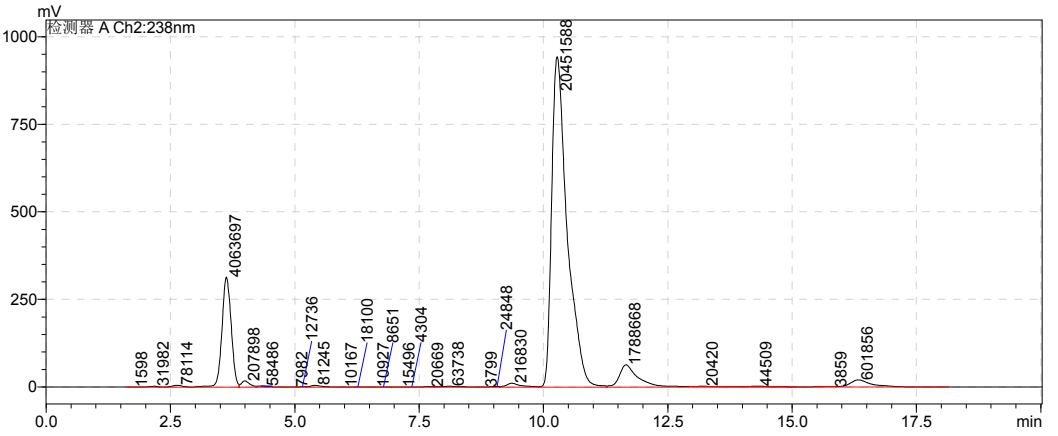


Figure S17 The HPLC spectrum of entry 10 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.271	20451588	25.0	**99 %**
1a	11.655	1788668		

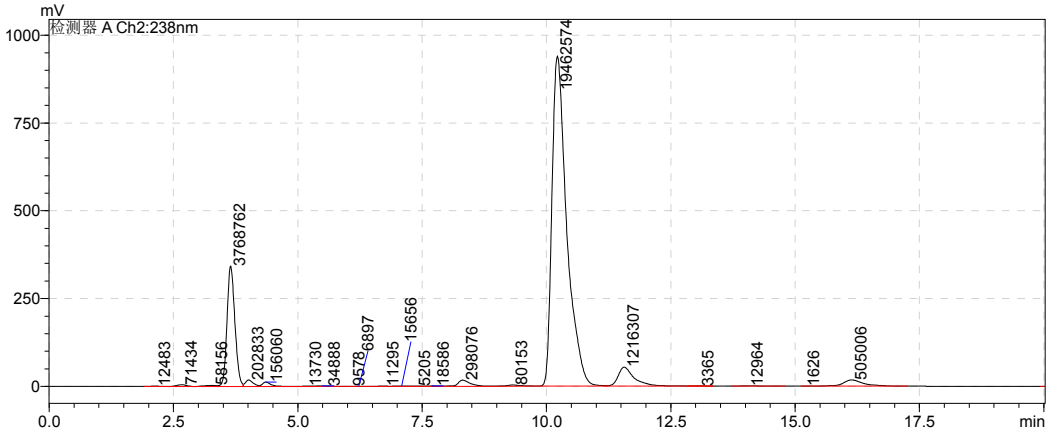


Figure S18 The HPLC spectrum of entry 11 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.215	19462574	23.8	**94 %**
1a	11.558	1216307		

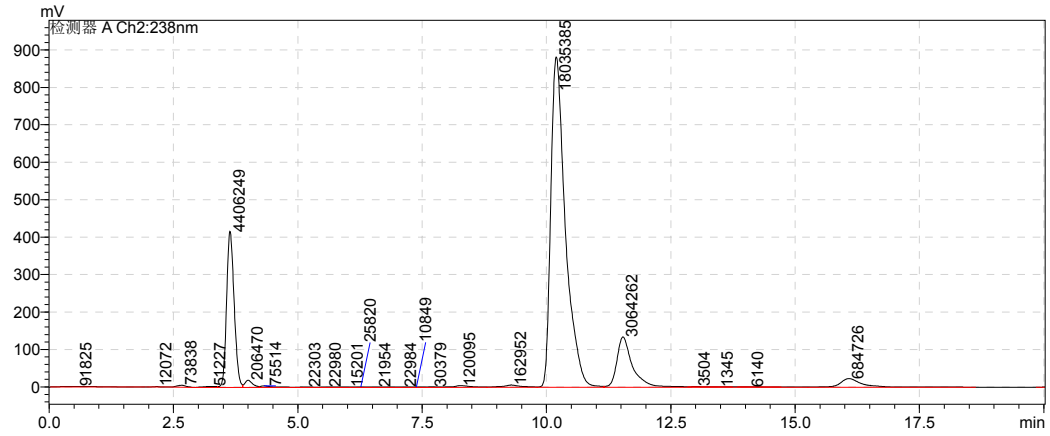


Figure S19 The HPLC spectrum of entry 12 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.192	18035385	20.0	**87 %**
1a	11.533	3064262		

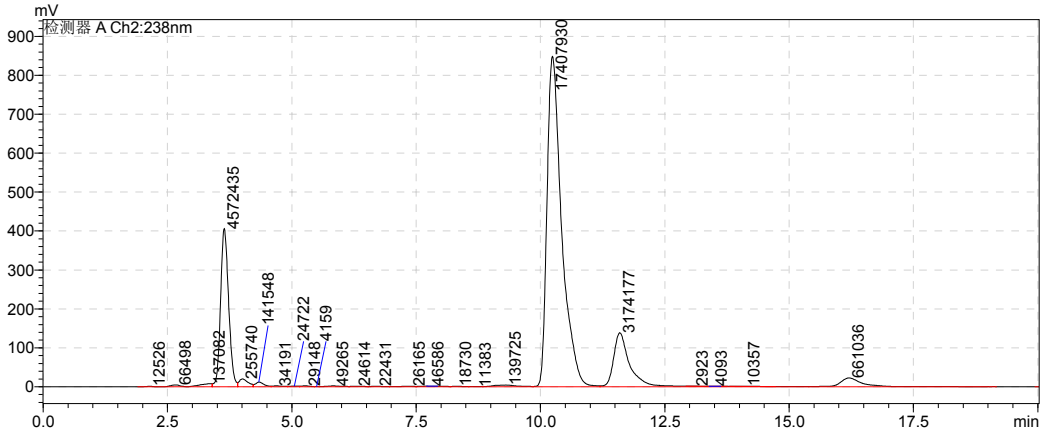


Figure S20 The HPLC spectrum of entry 13 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.237	17407930	21.2	**84 %**
1a	11.590	3174177		

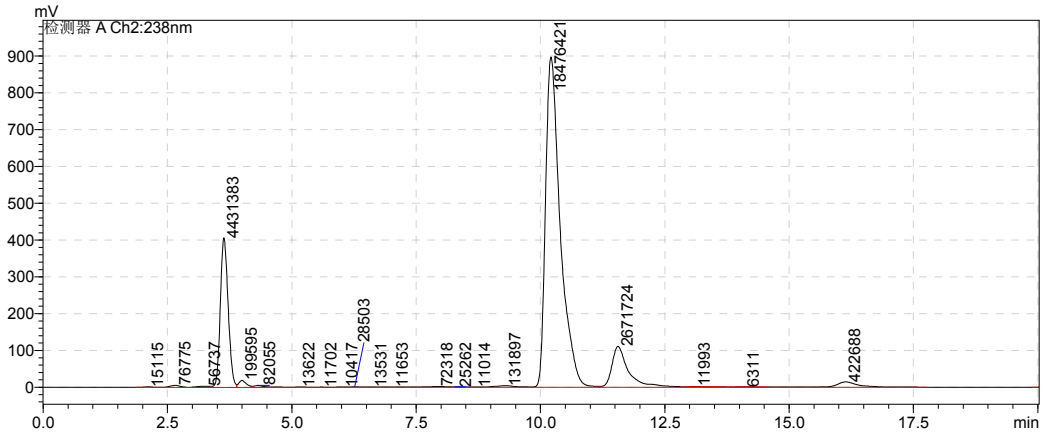


Figure S21 The HPLC spectrum of entry 14 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.207	18476421	22.7	**90 %**
1a	11.554	2671724		

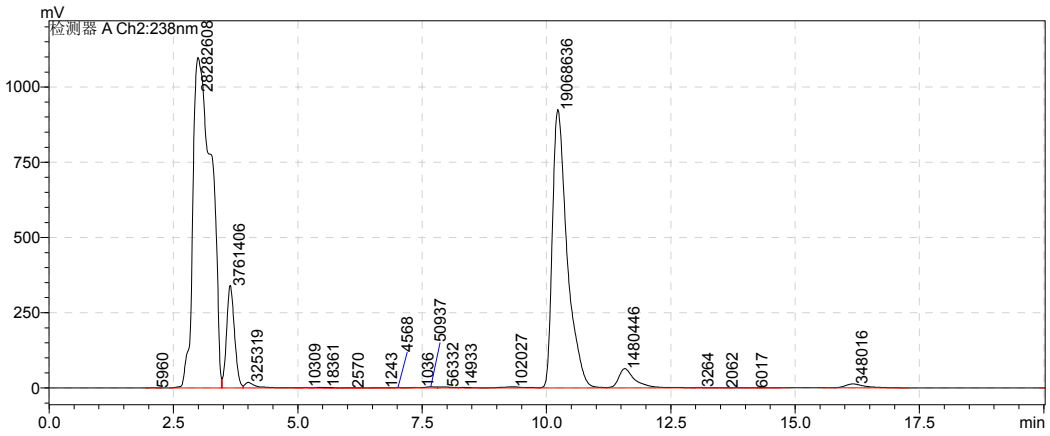


Figure S22 The HPLC spectrum of entry 15 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.224	19068636	23.3	**92 %**
1a	11.570	3174177		

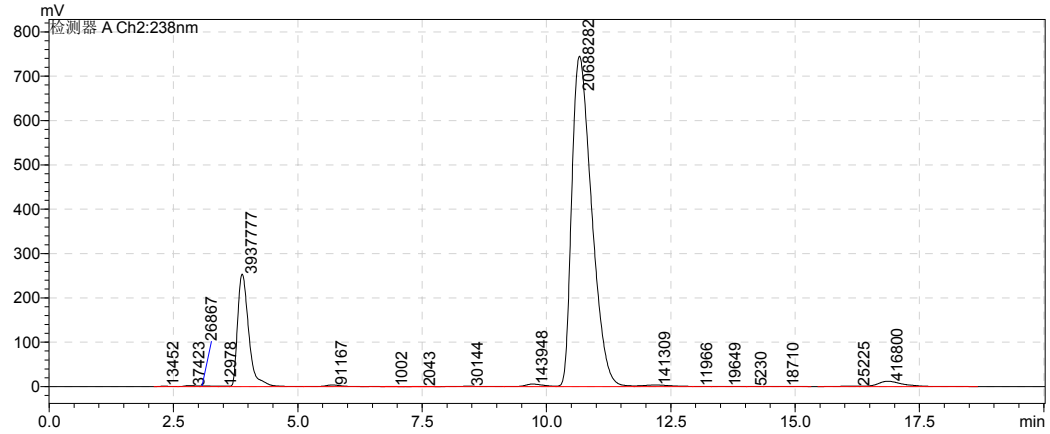


Figure S23 The HPLC spectrum of entry 16 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.659	20688282	25.3	**99 %**
1a	12.189	141309		

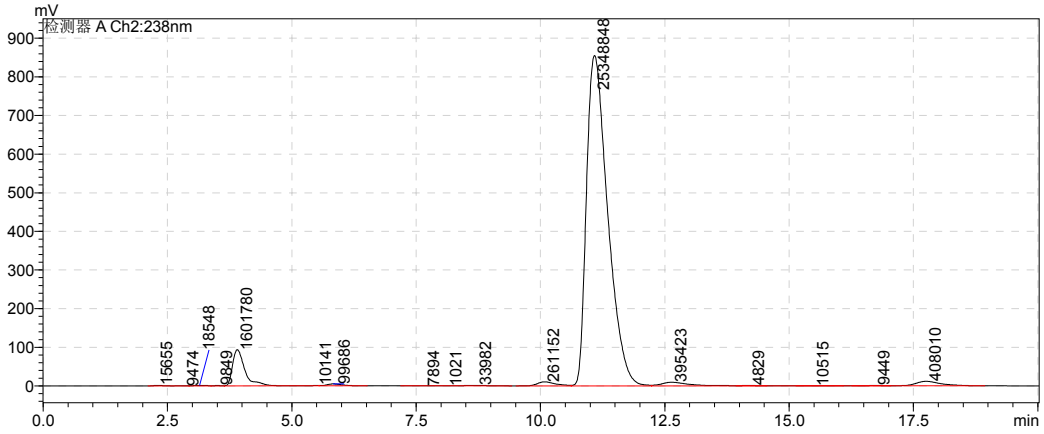


Figure S24 The HPLC spectrum of entry 17 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.682	25348848	62.4	**99 %**
1a	12.234	395423		

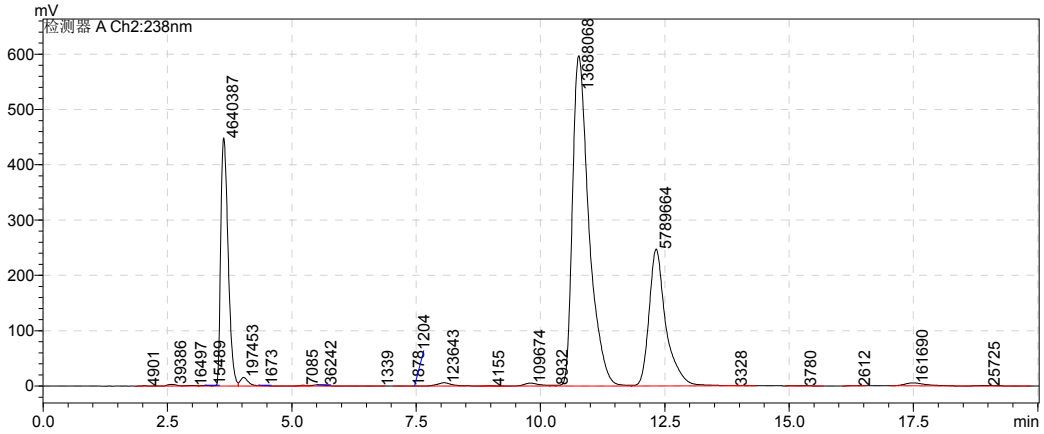


Figure S25 The HPLC spectrum of entry 18 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.466	13688068	16.6	**66 %**
1a	12.022	5789664		

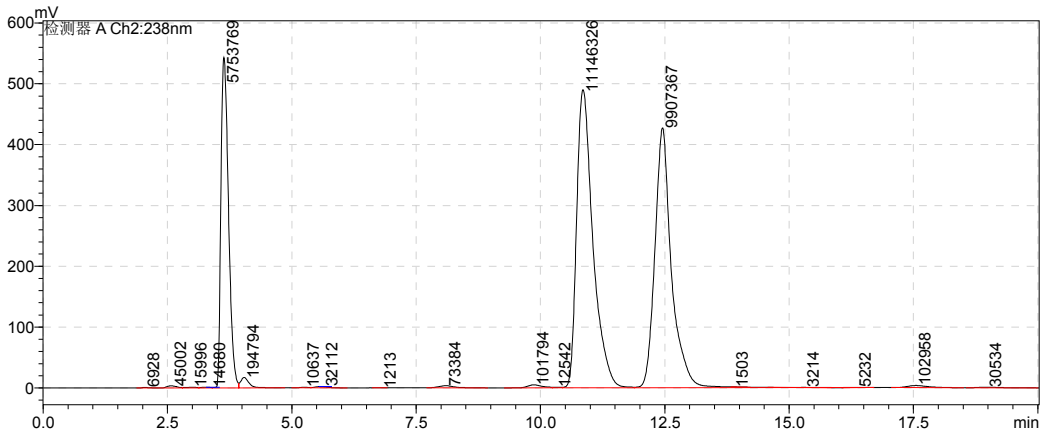


Figure S26 The HPLC spectrum of entry 19 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.502	11146326	13.4	**53 %**
1a	12.150	9907367		

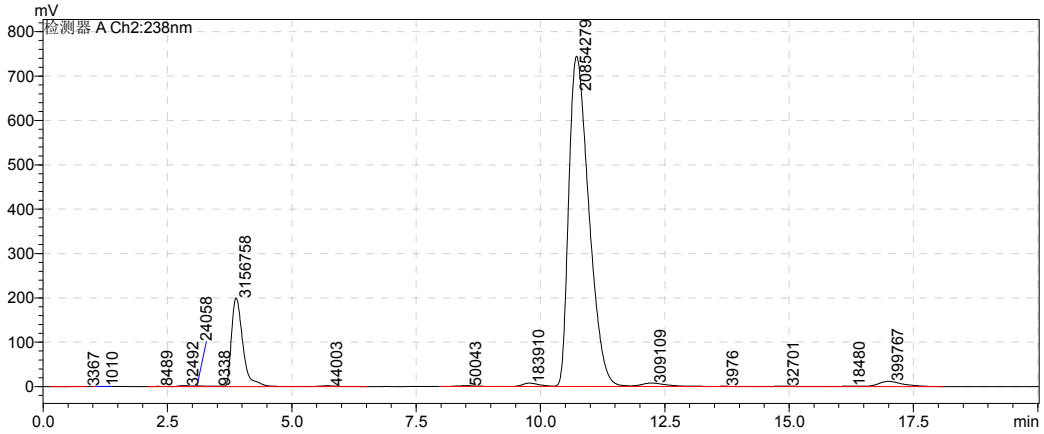


Figure S27 The HPLC spectrum of entry 20 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.422	20854279	25.5	**100 %**
1a	12.022	309109		

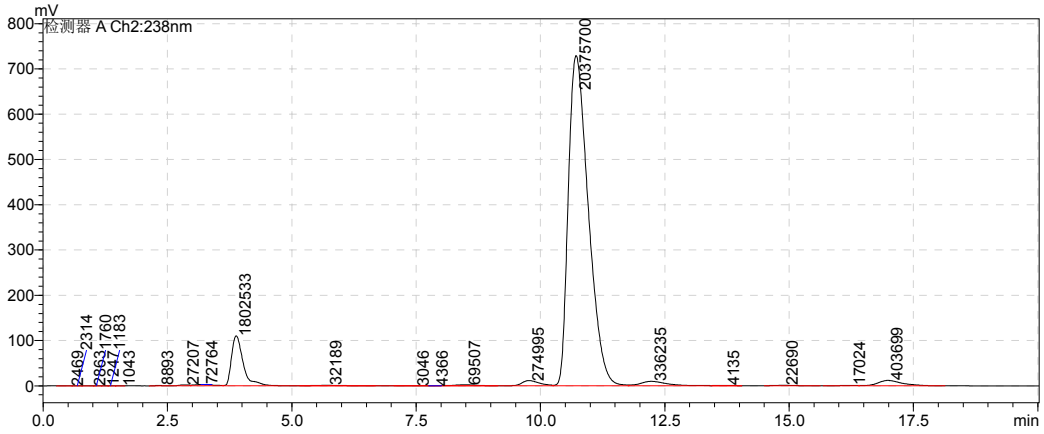


Figure S28 The HPLC spectrum of entry 21 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	1	20375700	25.0	**99 %**
1a	2	336235		

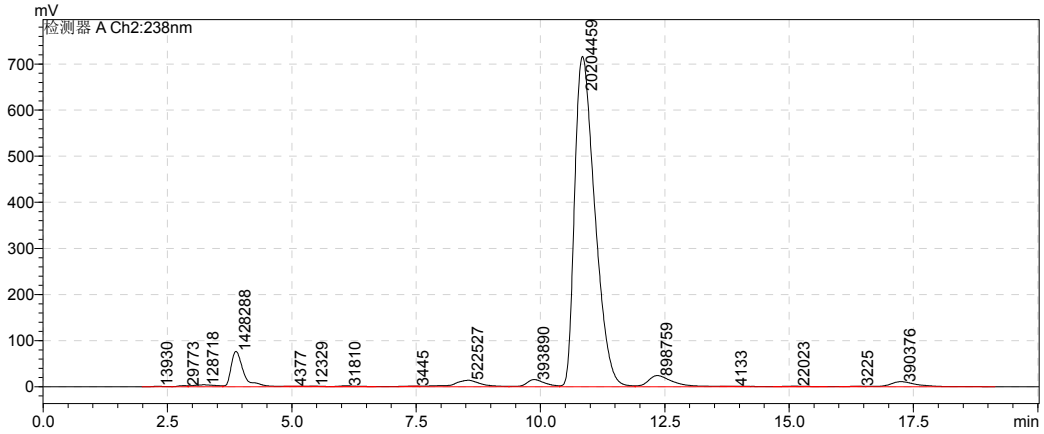


Figure S29 The HPLC spectrum of entry 22 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.440	20204459	24.7	**98 %**
1a	12.045	898759		

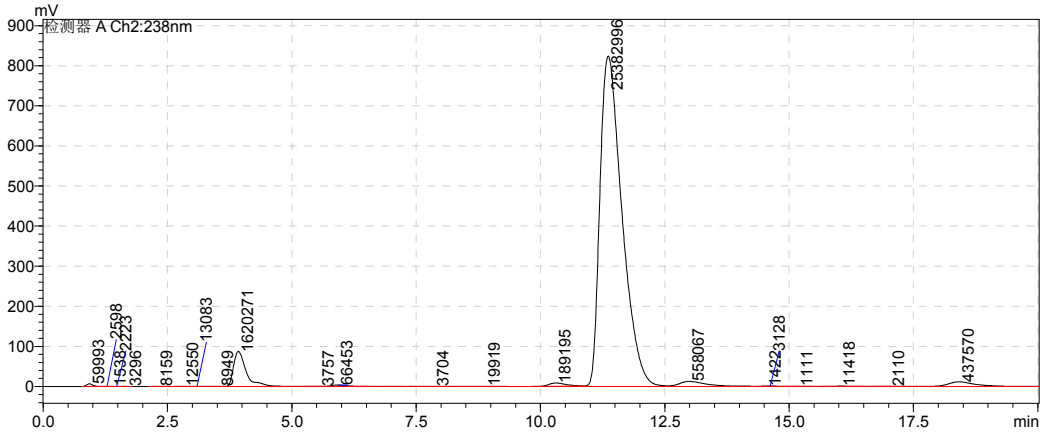


Figure S30 The HPLC spectrum of entry 23 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.857	25382996	124.9	**99 %**
1a	12.290	558067		

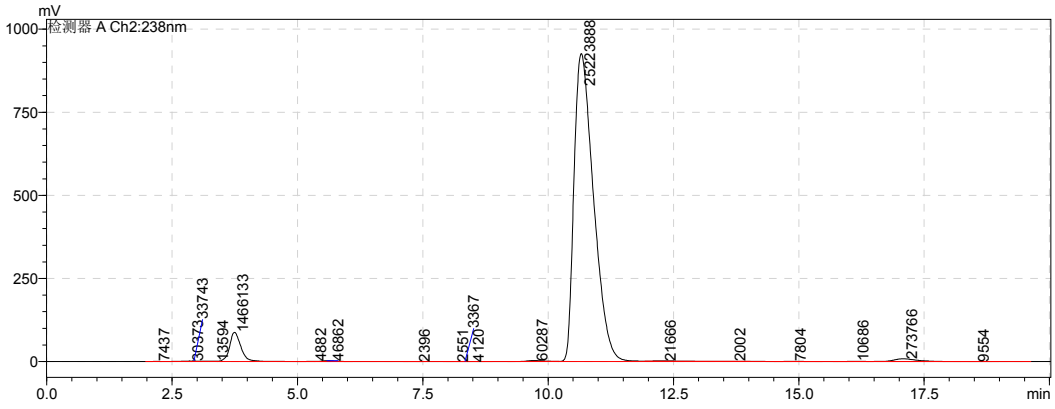
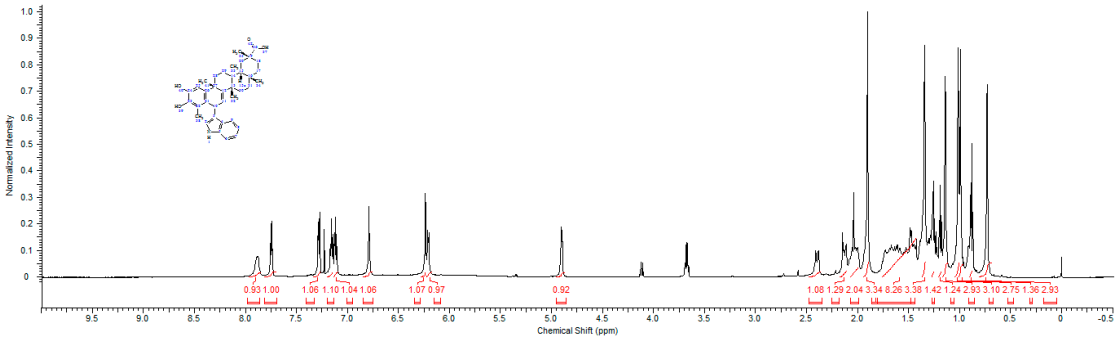


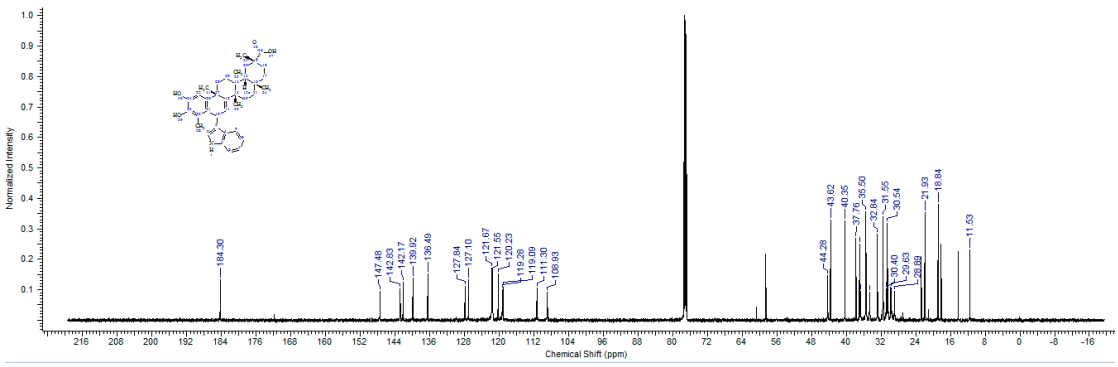
Figure S31 The HPLC spectrum of entry 24 in table 1

compound	Retention time	Peak area	Amount (mg)	Yield
2a	10.657	25223888	310.3	**98 %**
1a	12.270	21666		

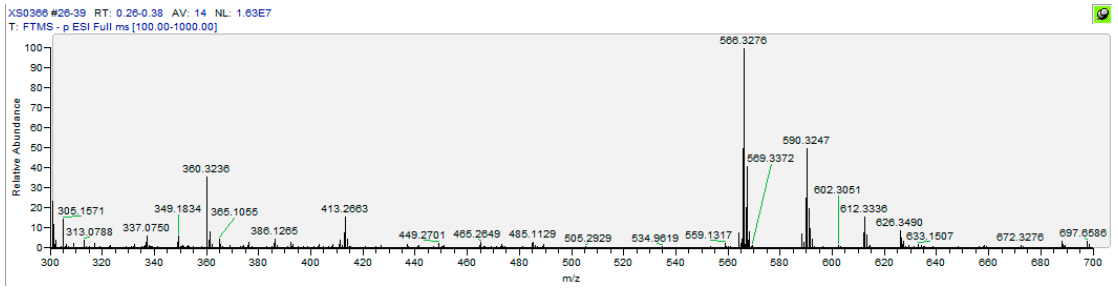
4. NMR spectra of synthesized compounds



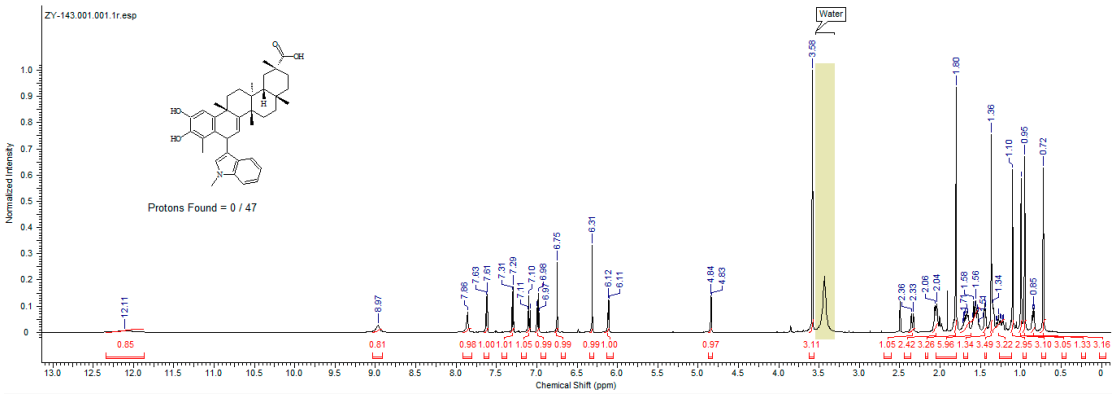
The ^{1}H NMR spectrum of compound 3a



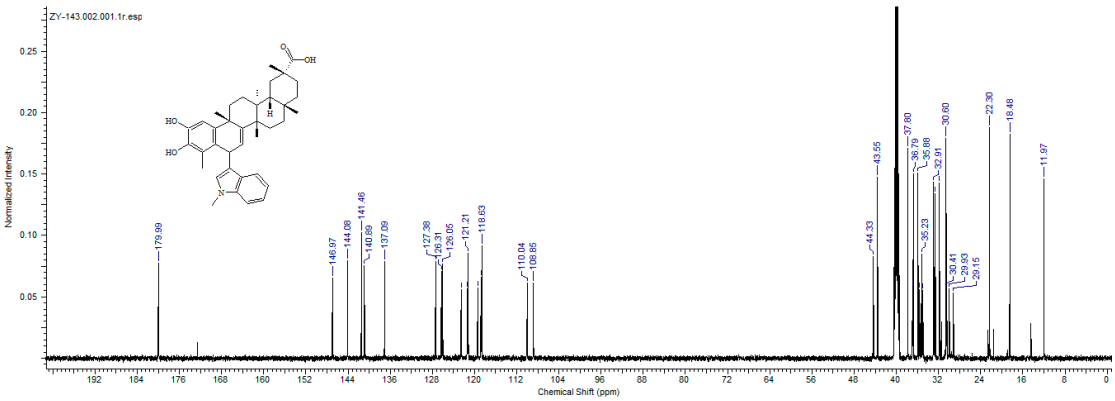
The ^{13}C NMR spectrum of compound 3a



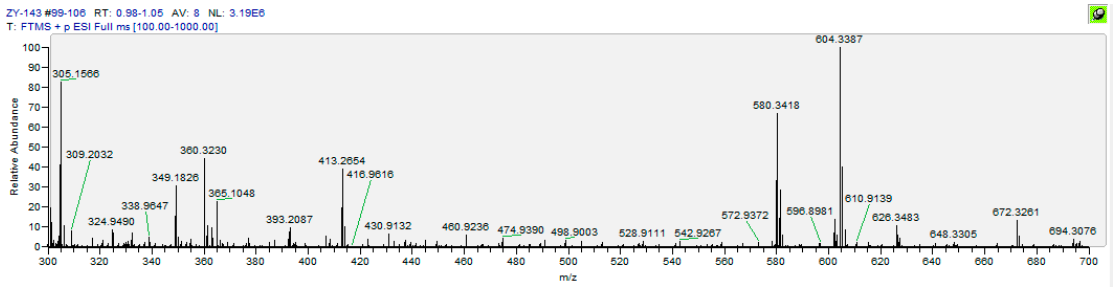
HRMS spectrum of compound 3a



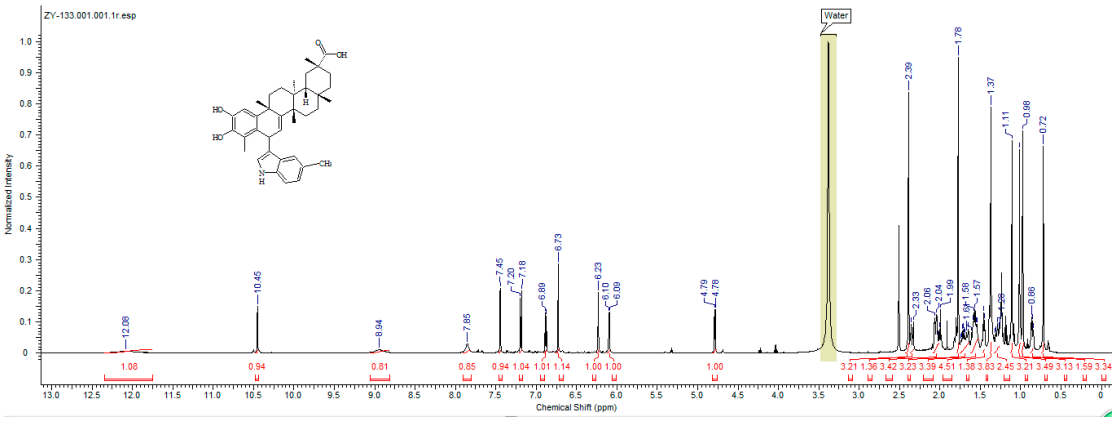
The ^{1}H NMR spectrum of compound 3b



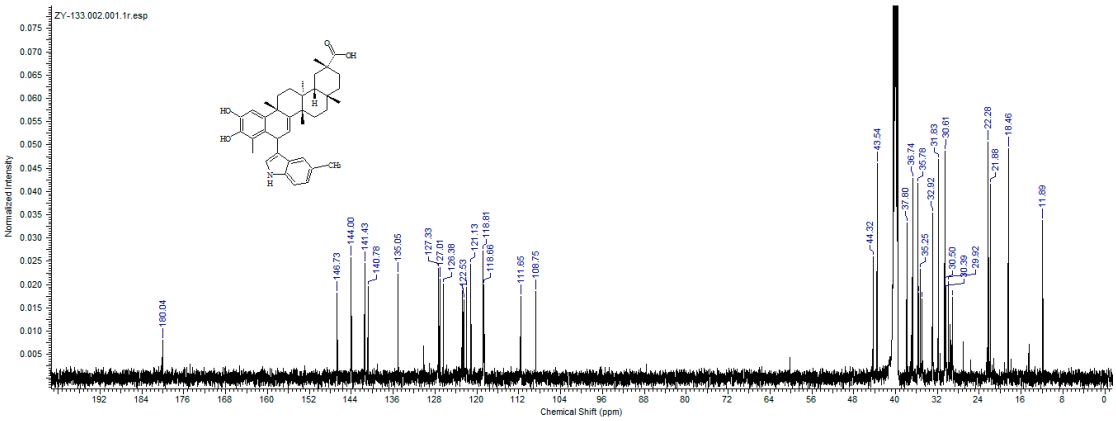
The ^{13}C NMR spectrum of compound 3b



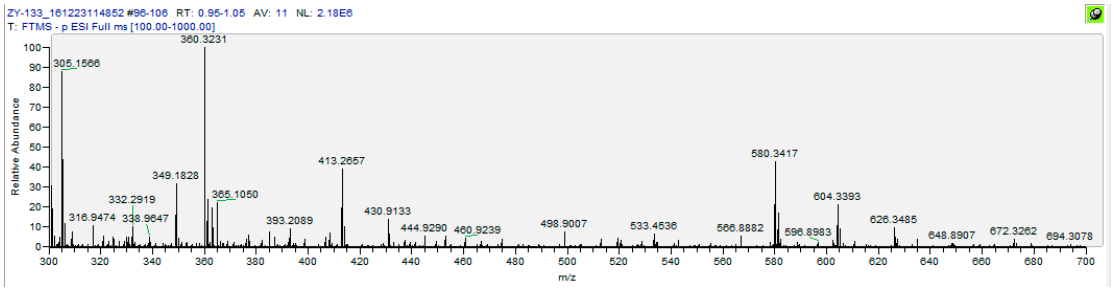
HRMS spectrum of compound 3b



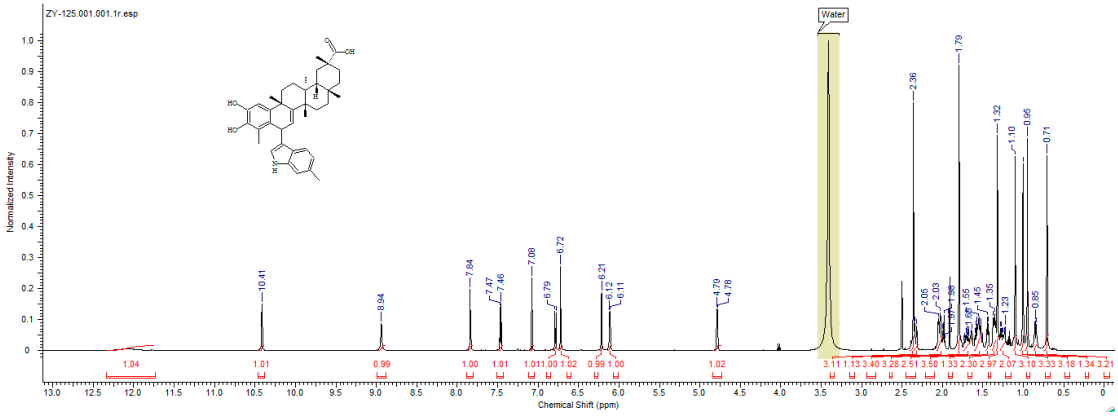
The ^{1}H NMR spectrum of compound 3c



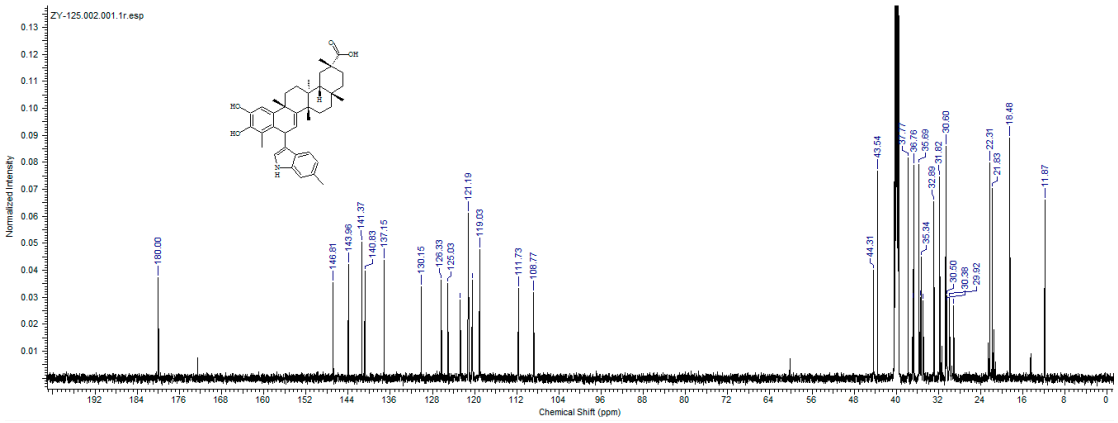
The ^{13}C NMR spectrum of compound 3c



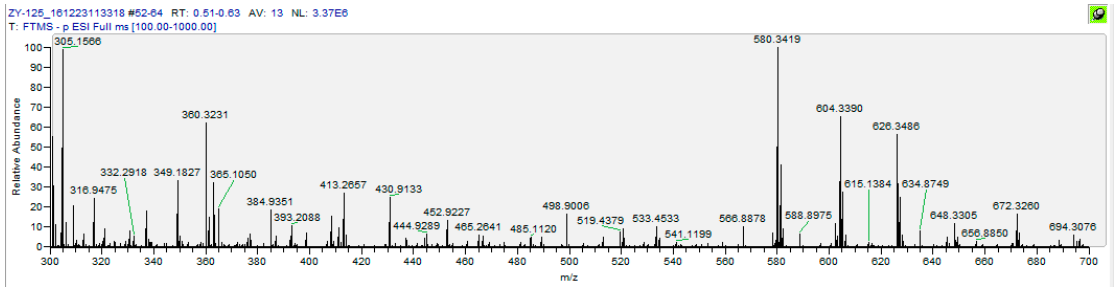
HRMS spectrum of compound 3c



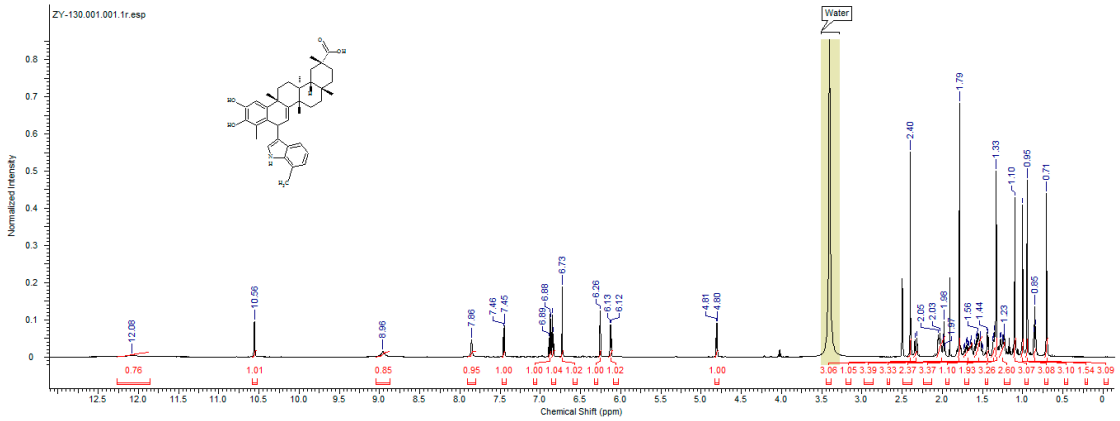
The ^{1}H NMR spectrum of compound 3d



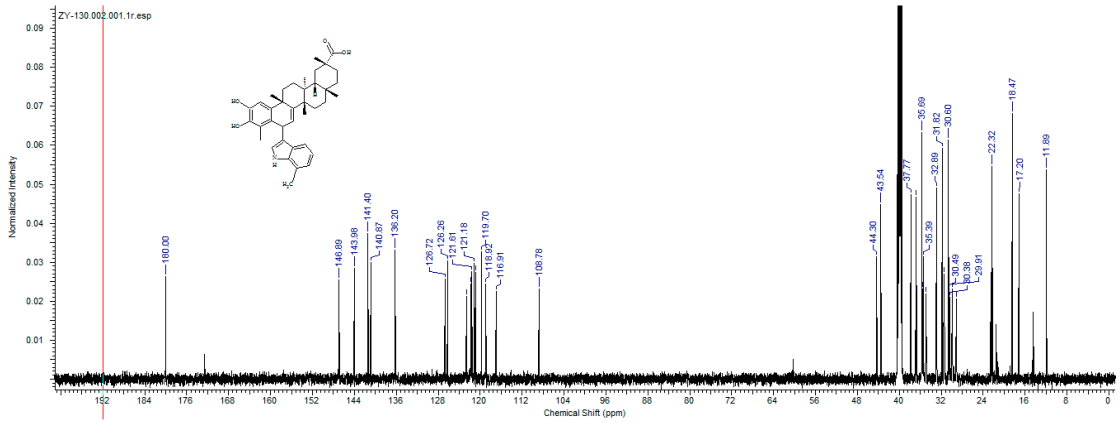
The ^{13}C NMR spectrum of compound 3d



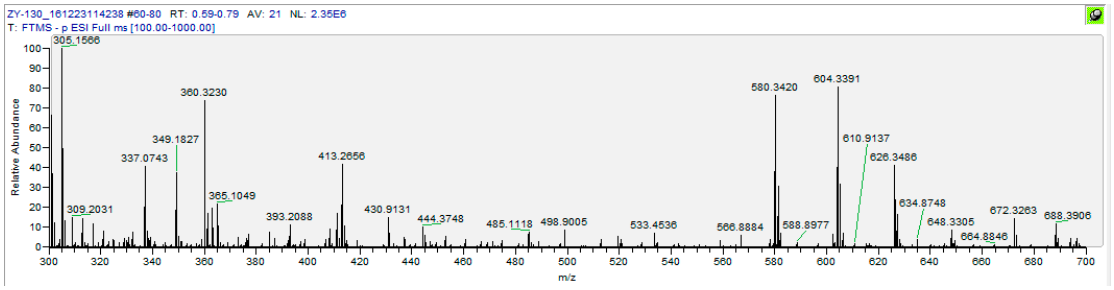
HRMS spectrum of compound 3d



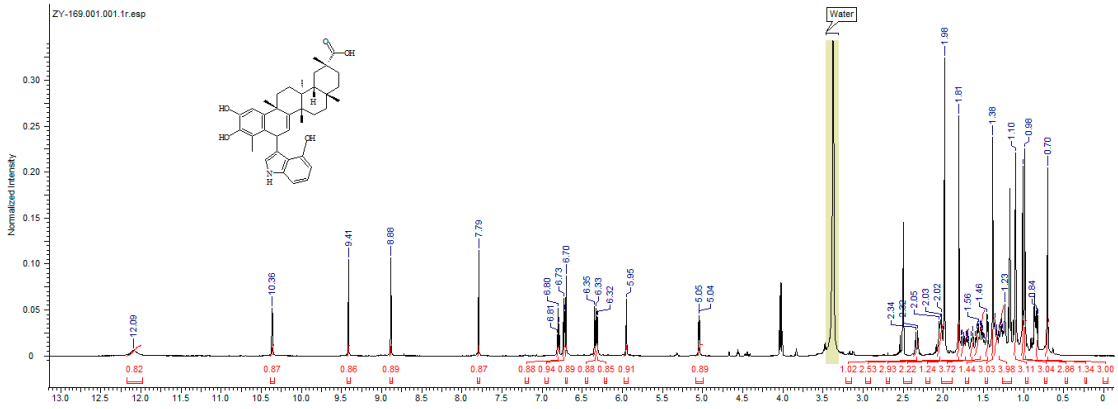
The ^{1}H NMR spectrum of compound 3e



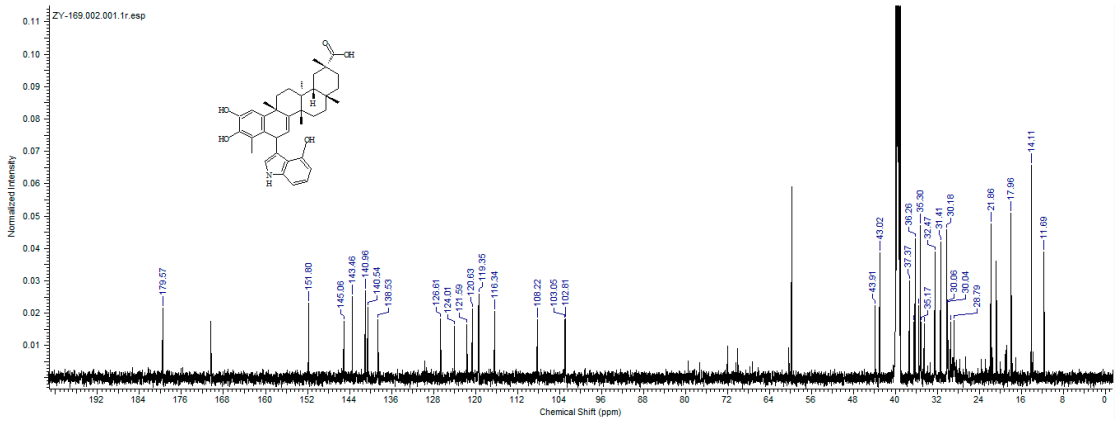
The ^{13}C NMR spectrum of compound 3e



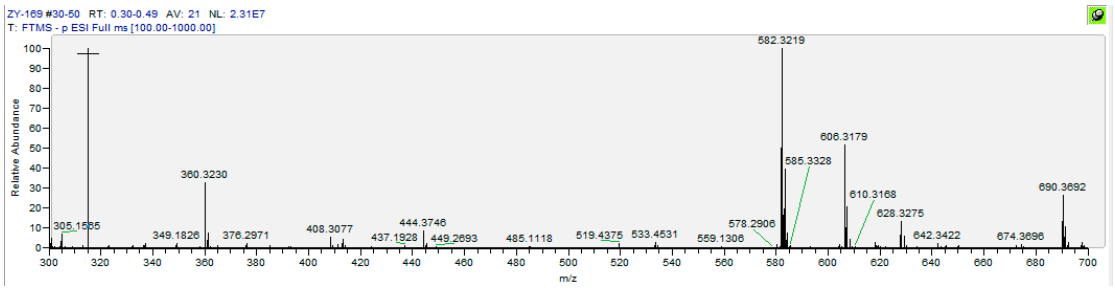
HRMS spectrum of compound 3e



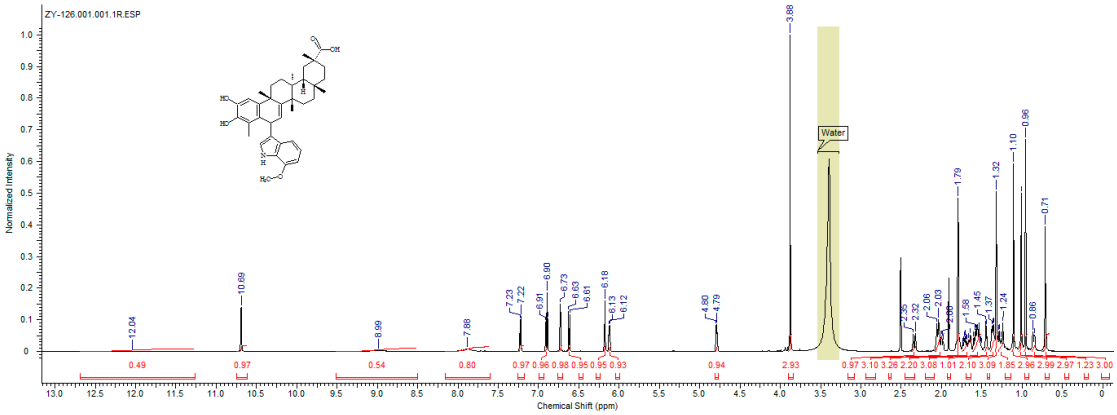
The ^{1}H NMR spectrum of compound 3f



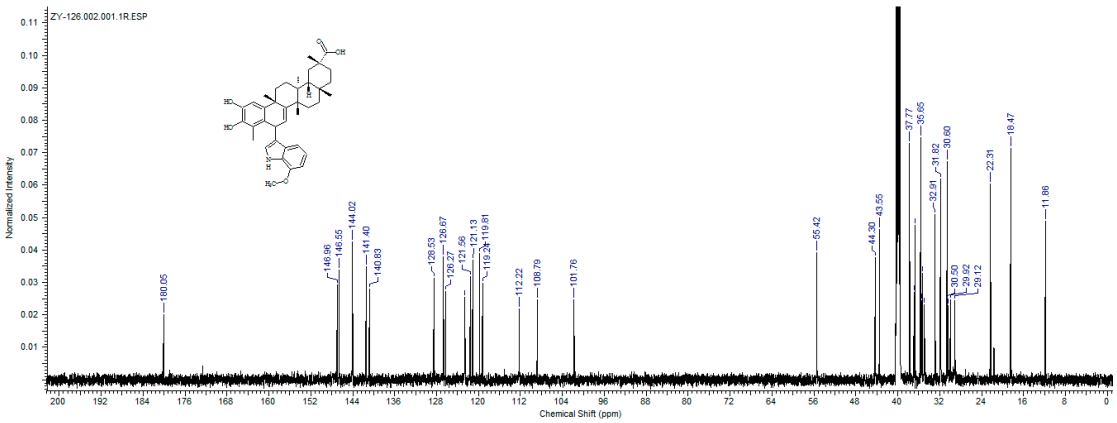
The ^{13}C NMR spectrum of compound 3f



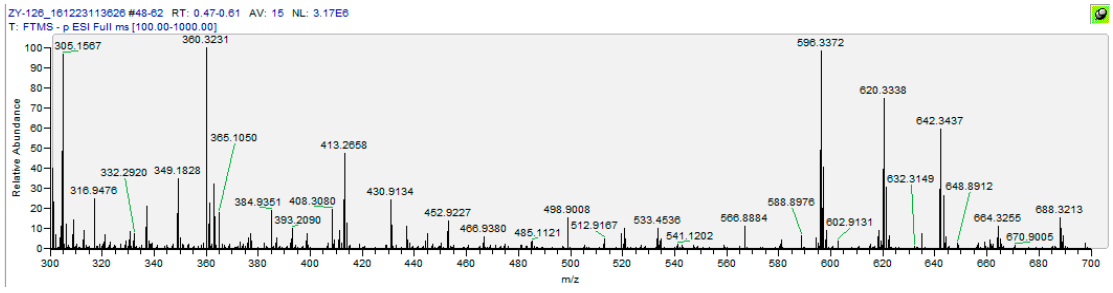
HRMS spectrum of compound 3f



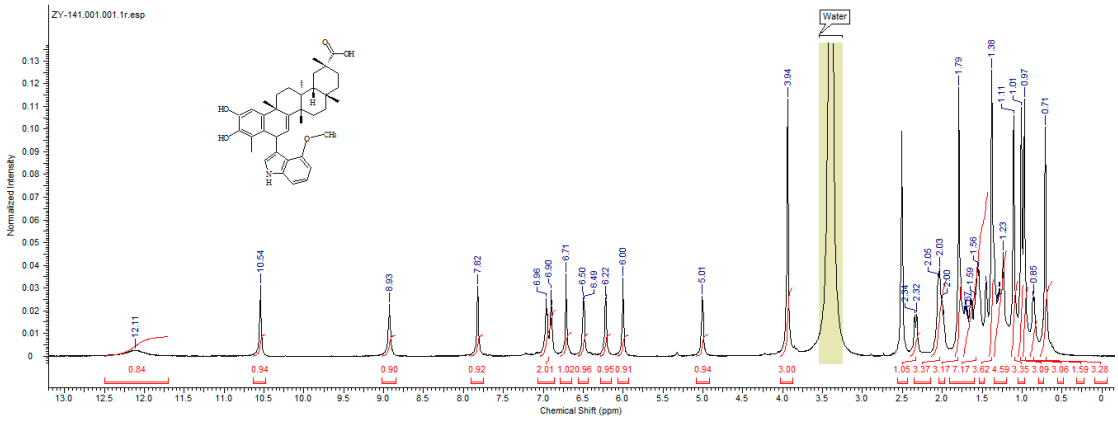
The ^{1}H NMR spectrum of compound 3h



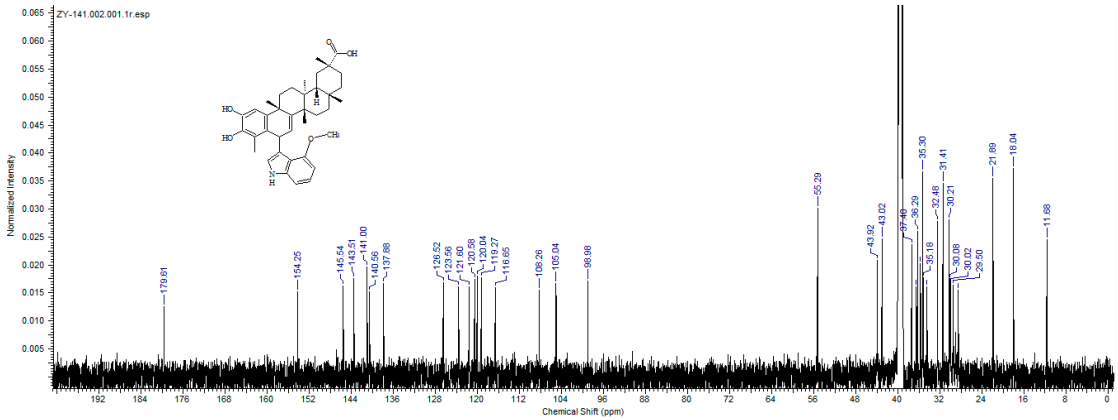
The ^{13}C NMR spectrum of compound 3h



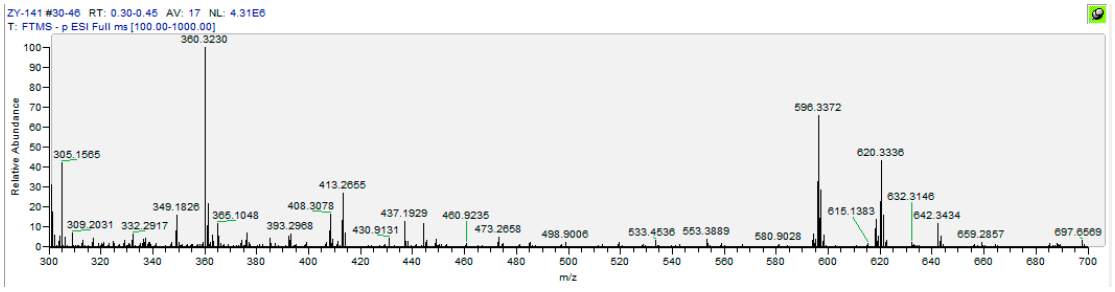
HRMS spectrum of compound 3h



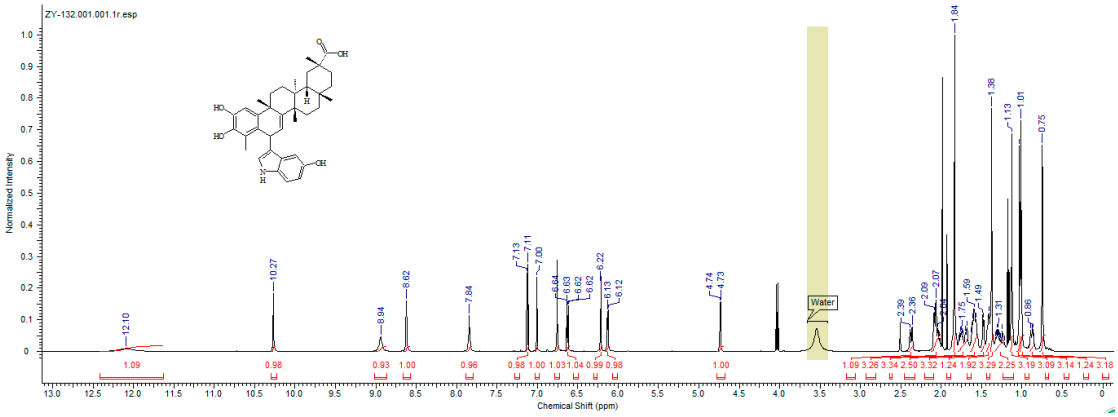
The ^{1}H NMR spectrum of compound 3i



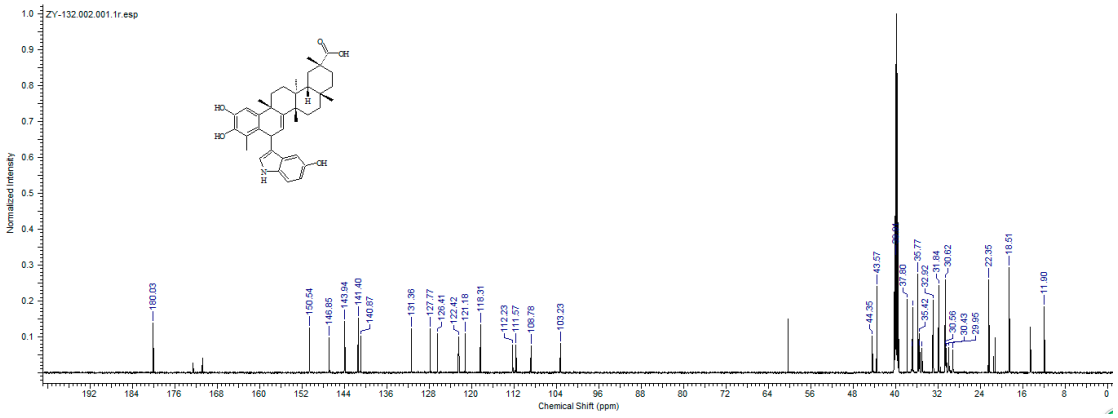
The ^{13}C NMR spectrum of compound 3i



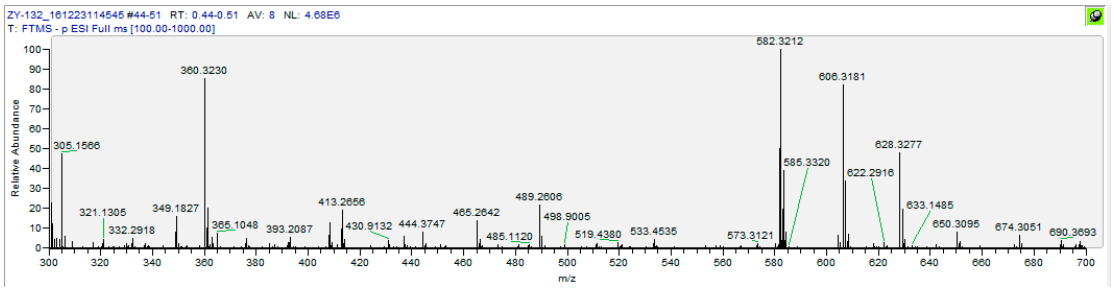
HRMS spectrum of compound 3i



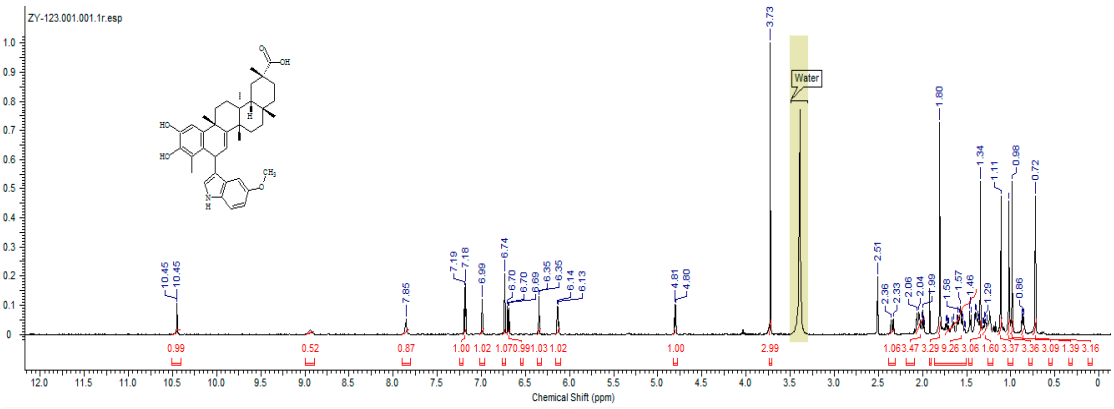
The ^{1}H NMR spectrum of compound 3j



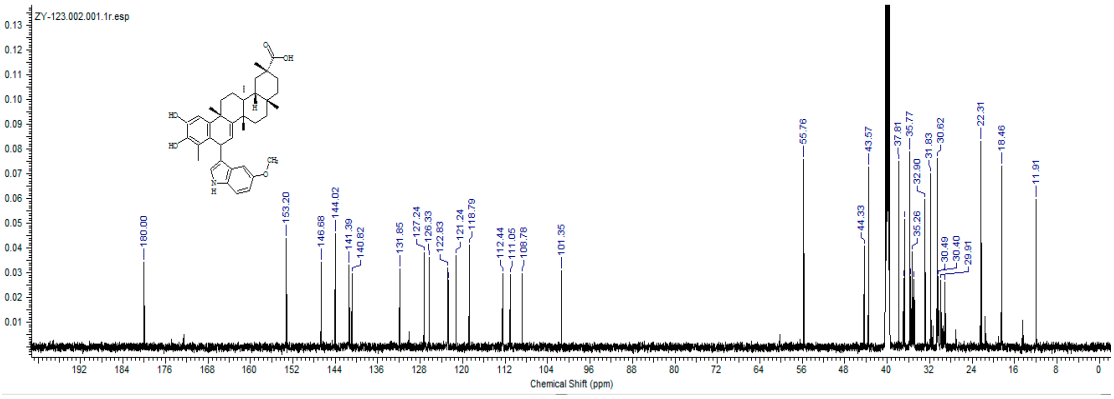
The ^{13}C NMR spectrum of compound 3j



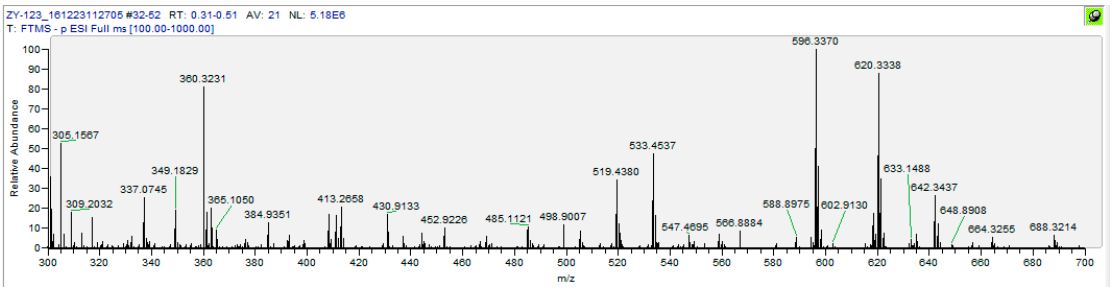
HRMS spectrum of compound 3j



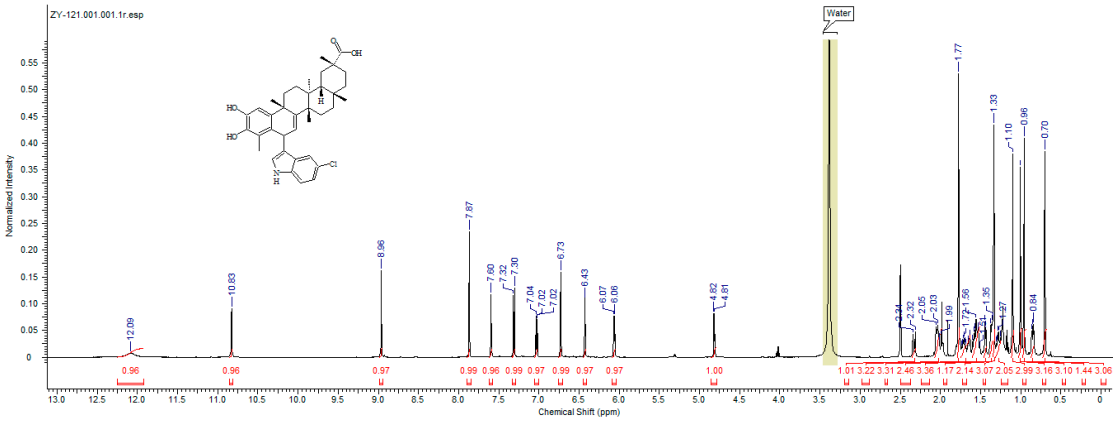
The ^{1}H NMR spectrum of compound 3k



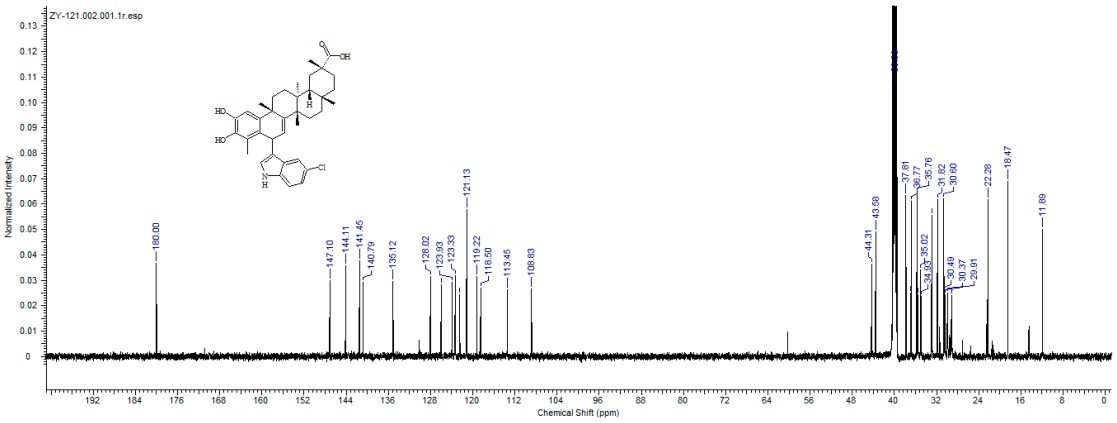
The ^{13}C NMR spectrum of compound 3k



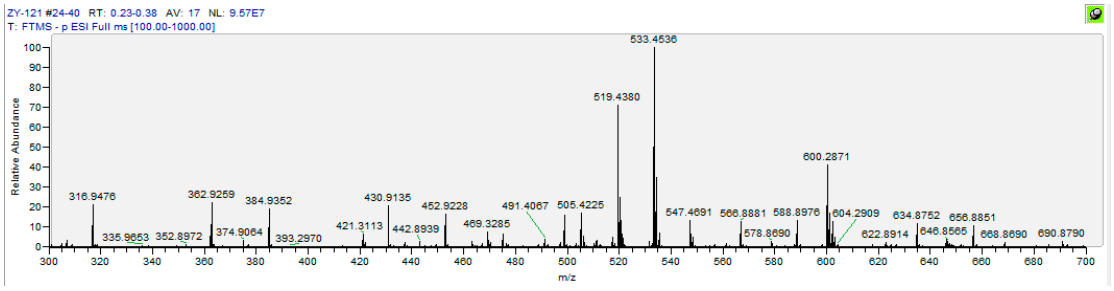
HRMS spectrum of compound 3k



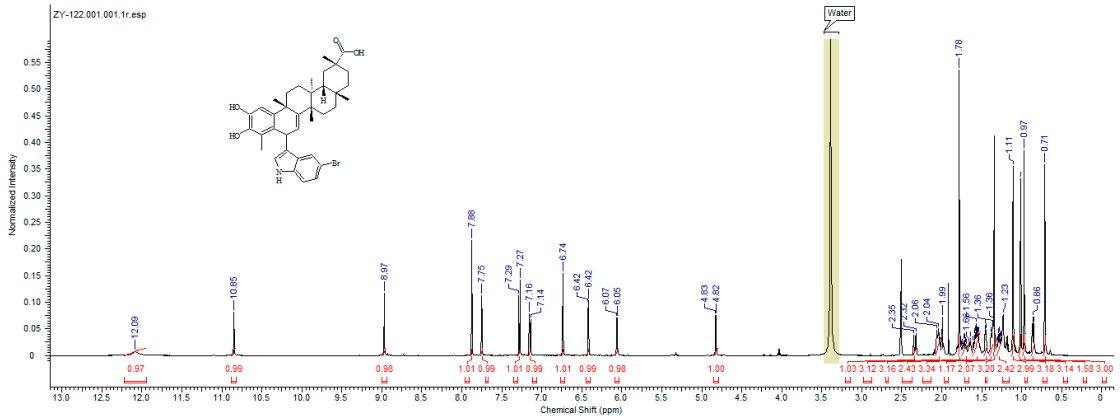
The ^{1}H NMR spectrum of compound 3l



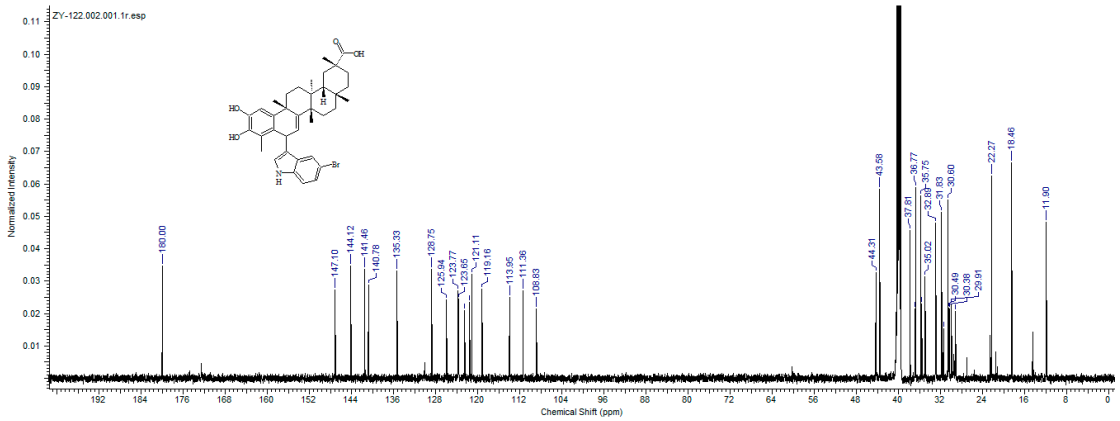
The ^{13}C NMR spectrum of compound 3l



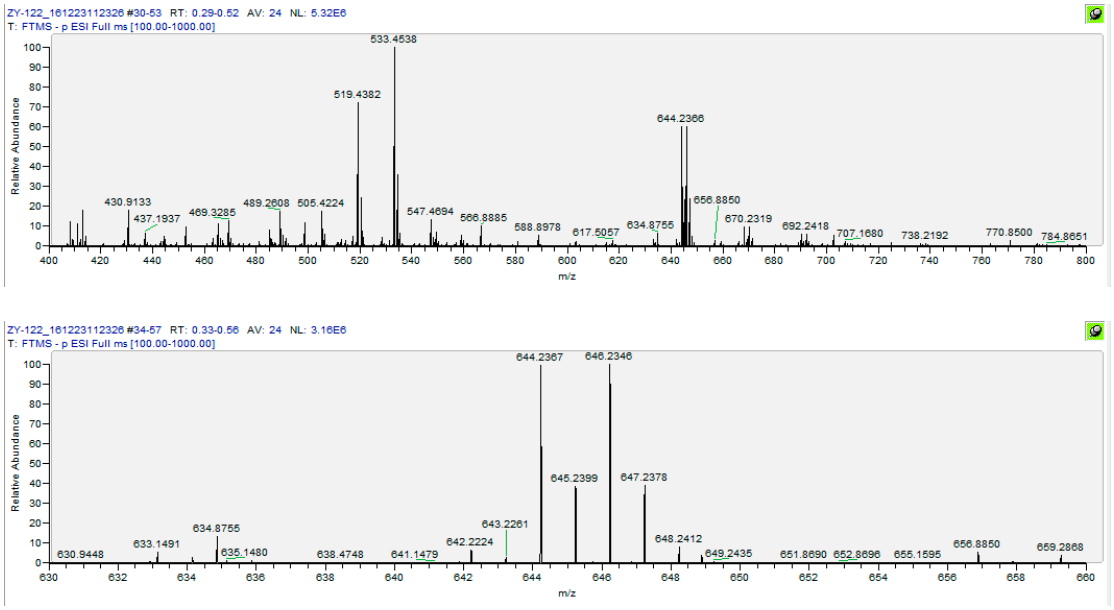
HRMS spectrum of compound 3l



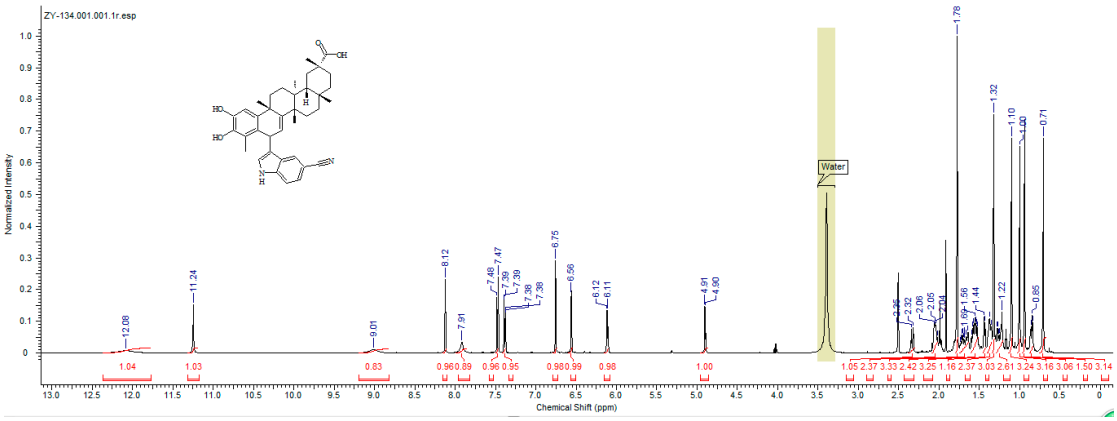
The ^{1}H NMR spectrum of compound 3m



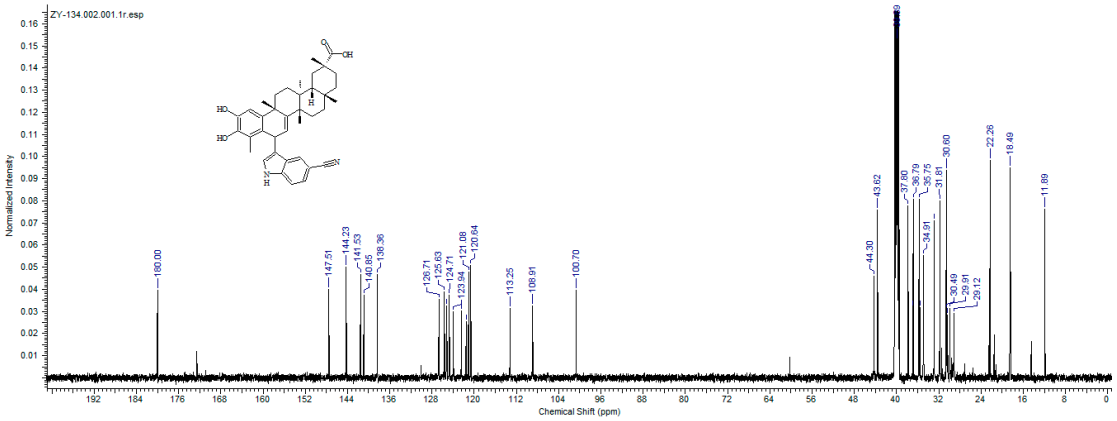
The ^{13}C NMR spectrum of compound 3m



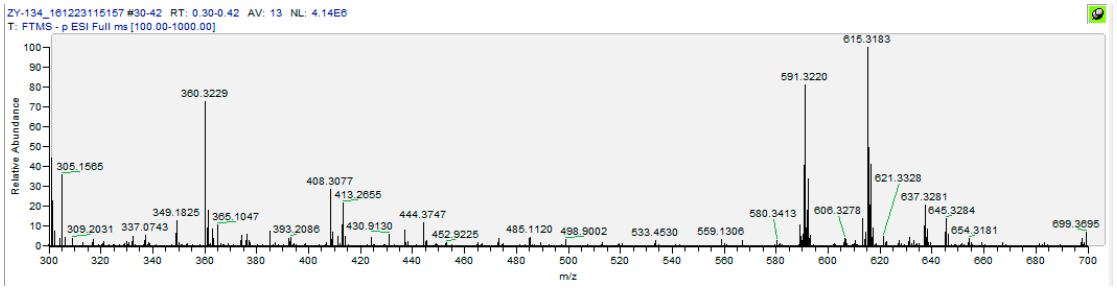
HRMS spectrum of compound 3m



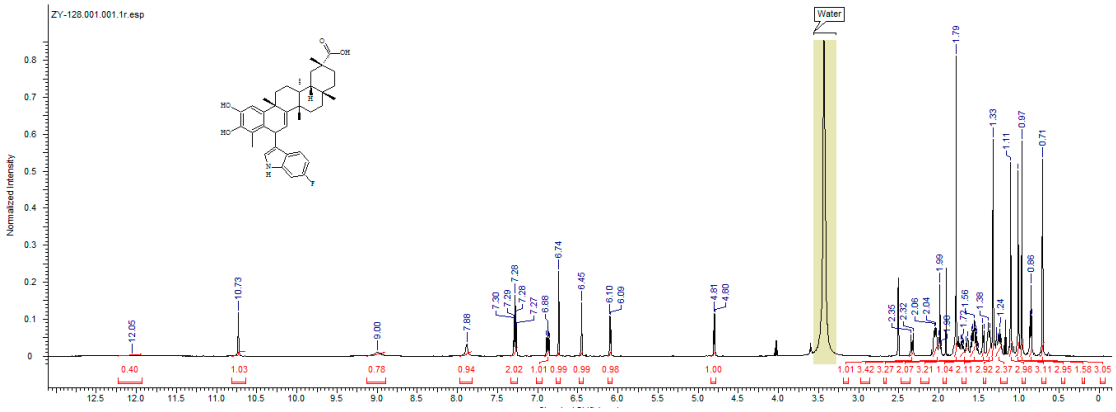
The ^{1}H NMR spectrum of compound 3n



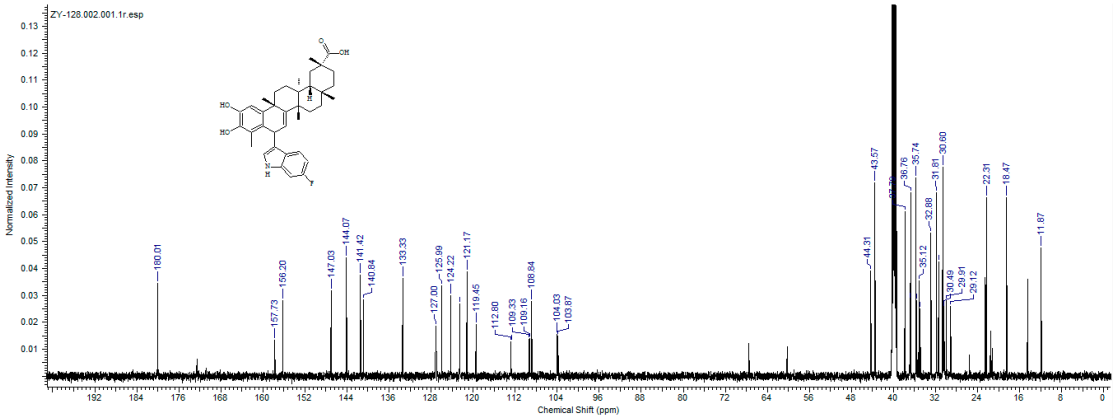
The ^{13}C NMR spectrum of compound 3n



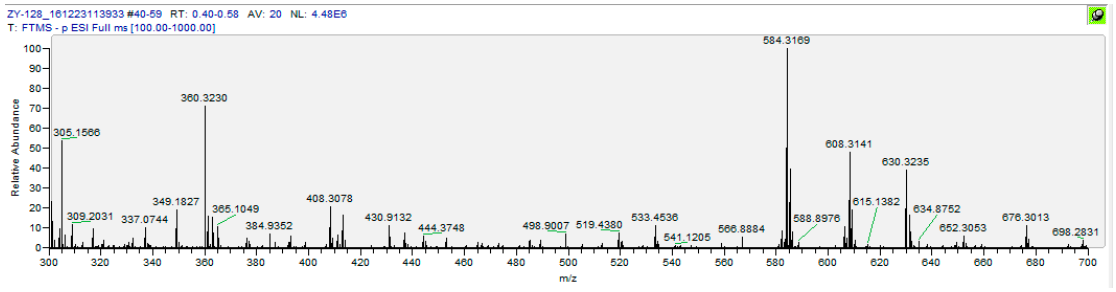
HRMS spectrum of compound 3n



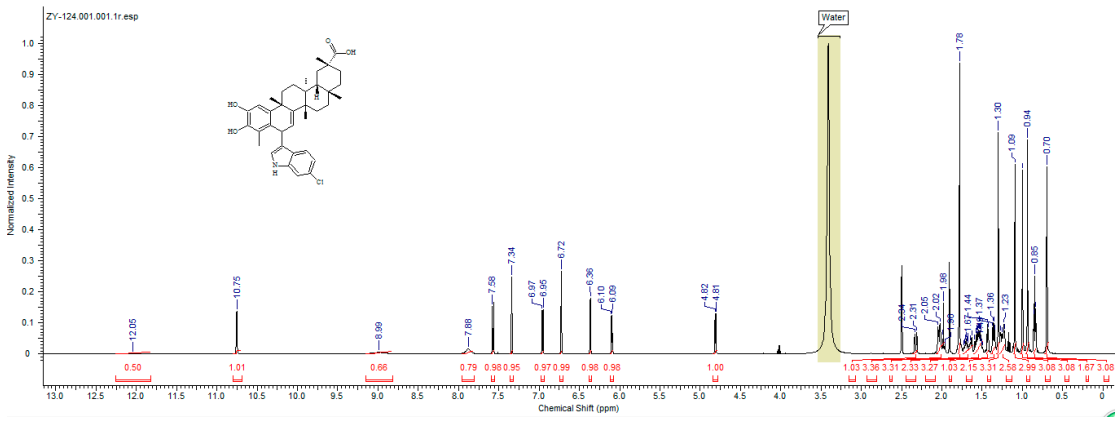
The ^{1}H NMR spectrum of compound 3o



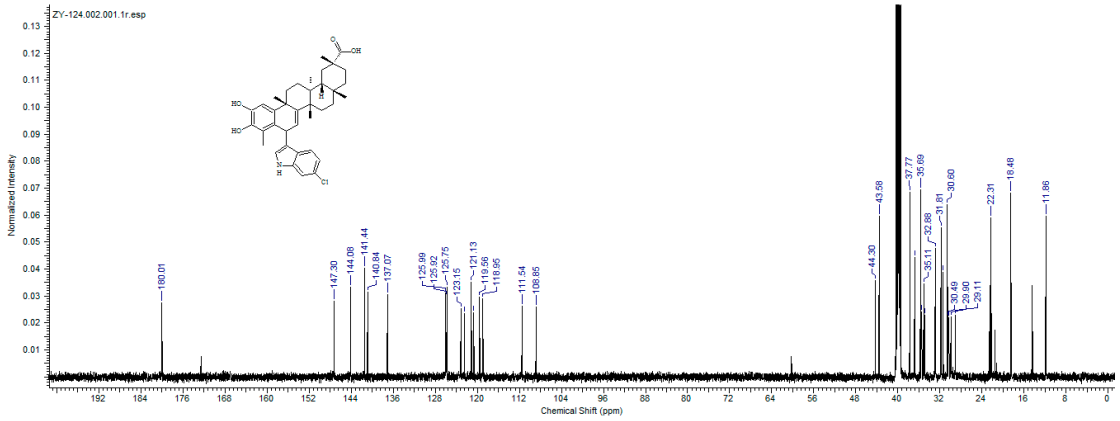
The ^{13}C NMR spectrum of compound 3o



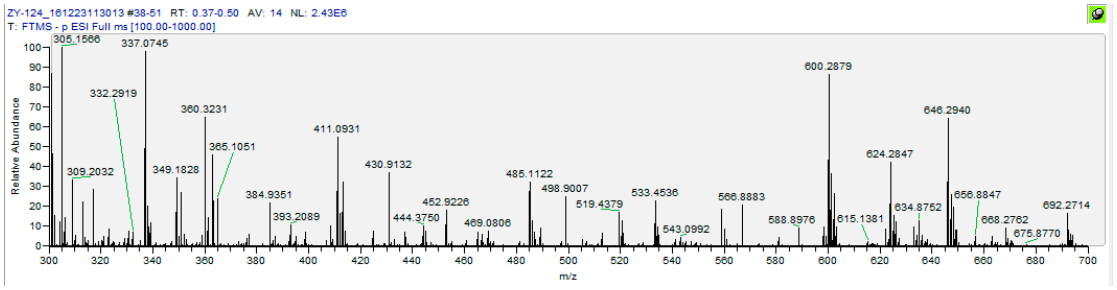
HRMS spectrum of compound 3o



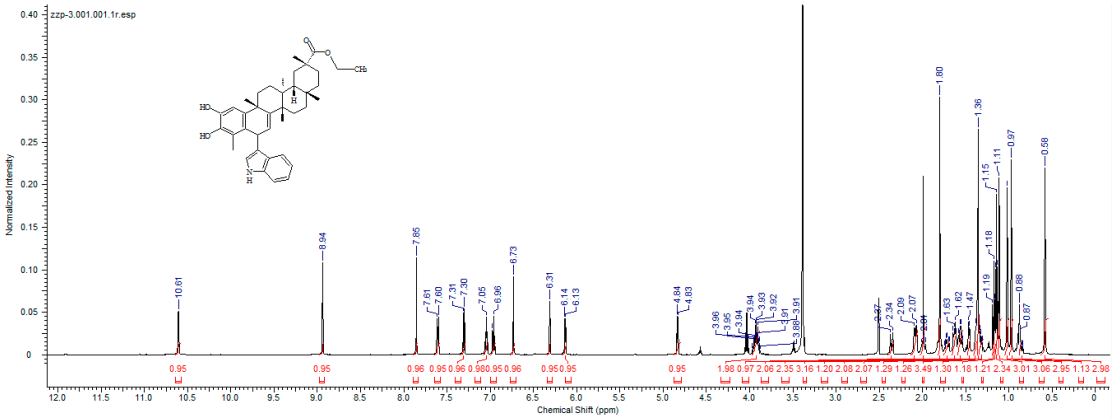
The ^{1}H NMR spectrum of compound 3p



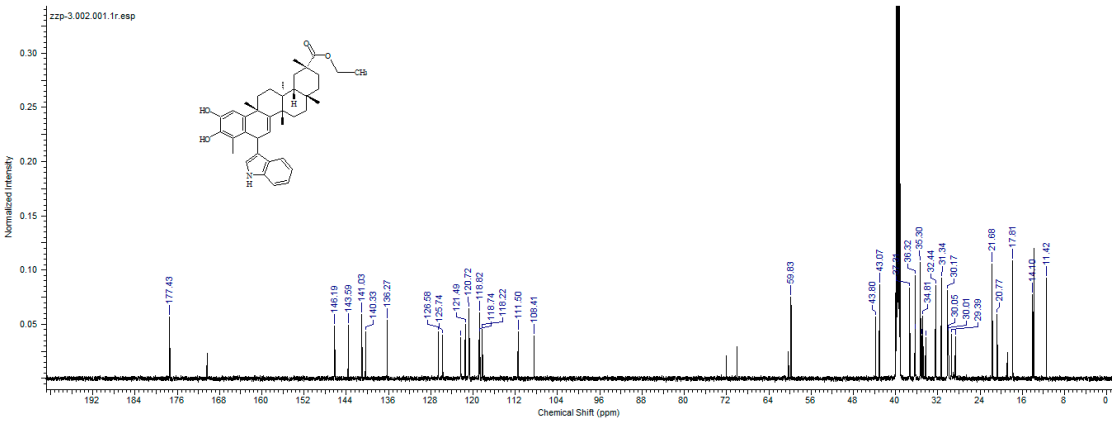
The ^{13}C NMR spectrum of compound 3p



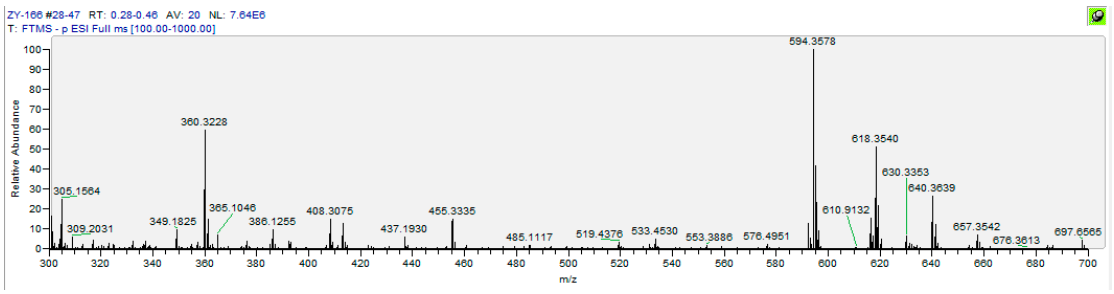
HRMS spectrum of compound 3p



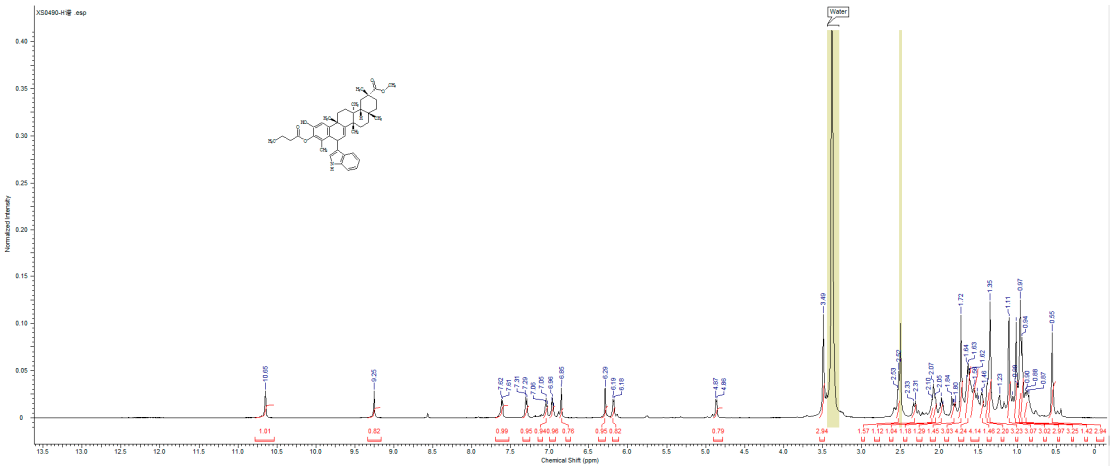
The ^{1}H NMR spectrum of compound 1a2b



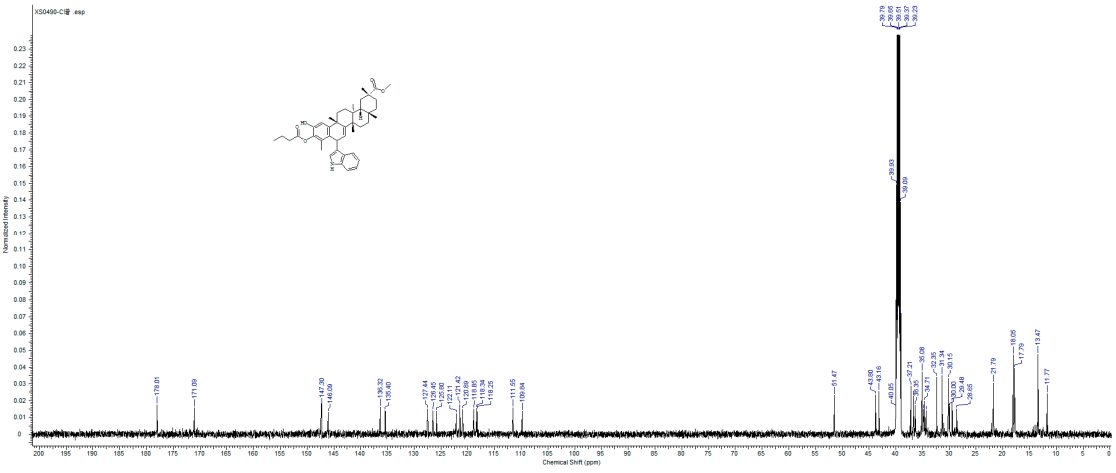
The ^{13}C NMR spectrum of compound 1a2b



HRMS spectrum of compound 1a2b



The ^{1}H NMR spectrum of compound 1a2c



The ^{13}C NMR spectrum of compound 1a2c