

Synthesis and Discovery of Andrographolide Derivatives as Nonsteroidal Farnesoid X Receptor (FXR) Antagonists

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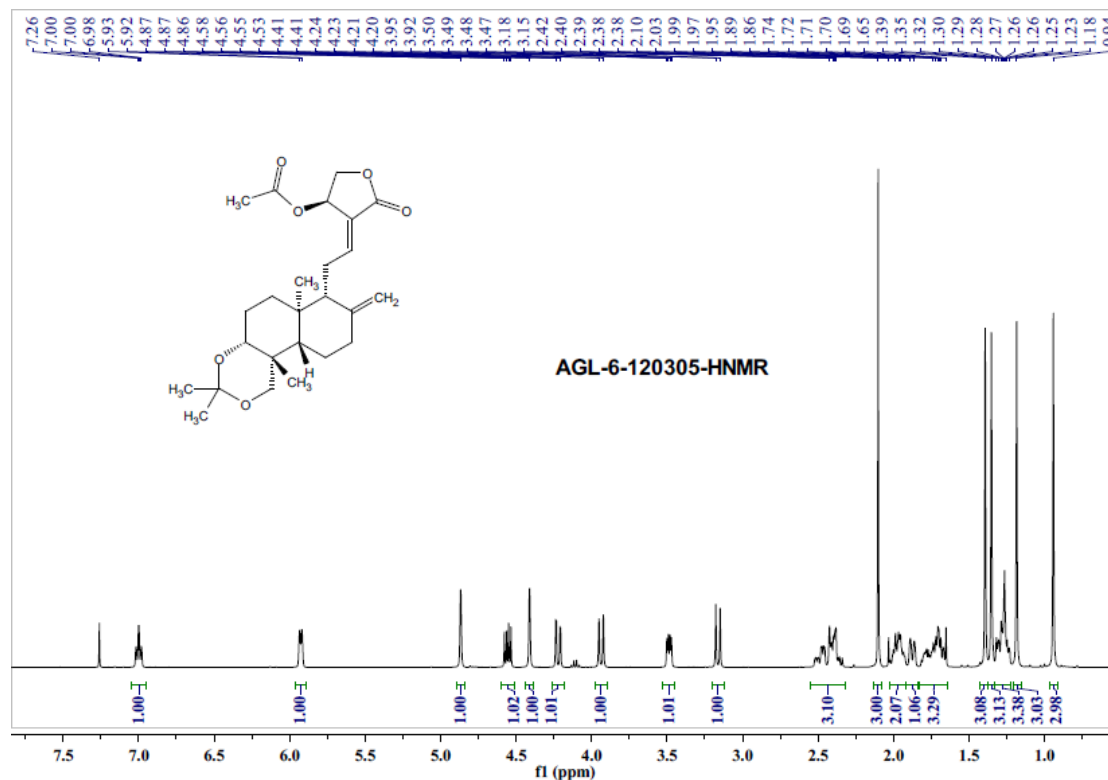
Table s1. Calculated Data of Lipinski's Rule of Five

entry	compd ^{a)}	R	14-isomer	MW	H-bond donors	H-bond acceptors	ClogP ^{b)}
1	10a	H	β	466.6	0	5	6.5108
2	12a	H	β	426.5	2	5	4.4698
3	10b	4'-NO ₂	β	511.6	0	8	6.5538
4	12b	4'-NO ₂	β	471.5	2	8	4.5128
5	10c	3'-NO ₂	β	511.6	0	8	6.5538
6	12c	3'-NO ₂	β	471.5	2	8	4.5128
7	10d	2'-NO ₂	β	511.6	0	8	6.5538
8	12d	2'-NO ₂	β	471.5	2	8	4.5128
9	10e	2'-CO ₂ Et	β	538.7	0	7	7.0238
10	12e	2'-CO ₂ Et	β	498.6	2	7	4.9828
11	10f	2'-OCH ₃	β	496.6	0	6	6.2498
12	12f	2'-OCH ₃	β	456.6	2	6	4.2088
13	10g	2'-OCH ₃ -4'-NO ₂	β	541.6	0	9	6.2723
14	12g	2'-OCH ₃ -4'-NO ₂	β	501.6	2	9	4.2313
15	10h	2'-CH ₃ -4'-NO ₂	β	525.6	0	8	7.0528
16	12h	2'-CH ₃ -4'-NO ₂	β	485.6	2	8	5.0118
17	10i	2'-F-4'-NO ₂	β	529.6	0	9	6.5458
18	12i	2'-F-4'-NO ₂	β	489.5	2	9	4.5048
19	11b	4'-NO ₂	α	511.6	0	8	6.5538
20	13b	4'-NO ₂	α	471.5	2	8	4.5128
21	11g	2'-OCH ₃ -4'-NO ₂	α	541.6	0	9	6.2723
22	13g	2'-OCH ₃ -4'-NO ₂	α	501.6	2	9	4.2313
23	1, andrographolide		α	350.4	3	5	2.1186
24	5		α	390.5	1	5	4.1598
25	6		β	432.5	0	6	5.0182
26	7		β	392.5	2	6	2.9772
27	8		β	350.4	3	5	2.1186
28	9		β	390.5	1	5	4.1598

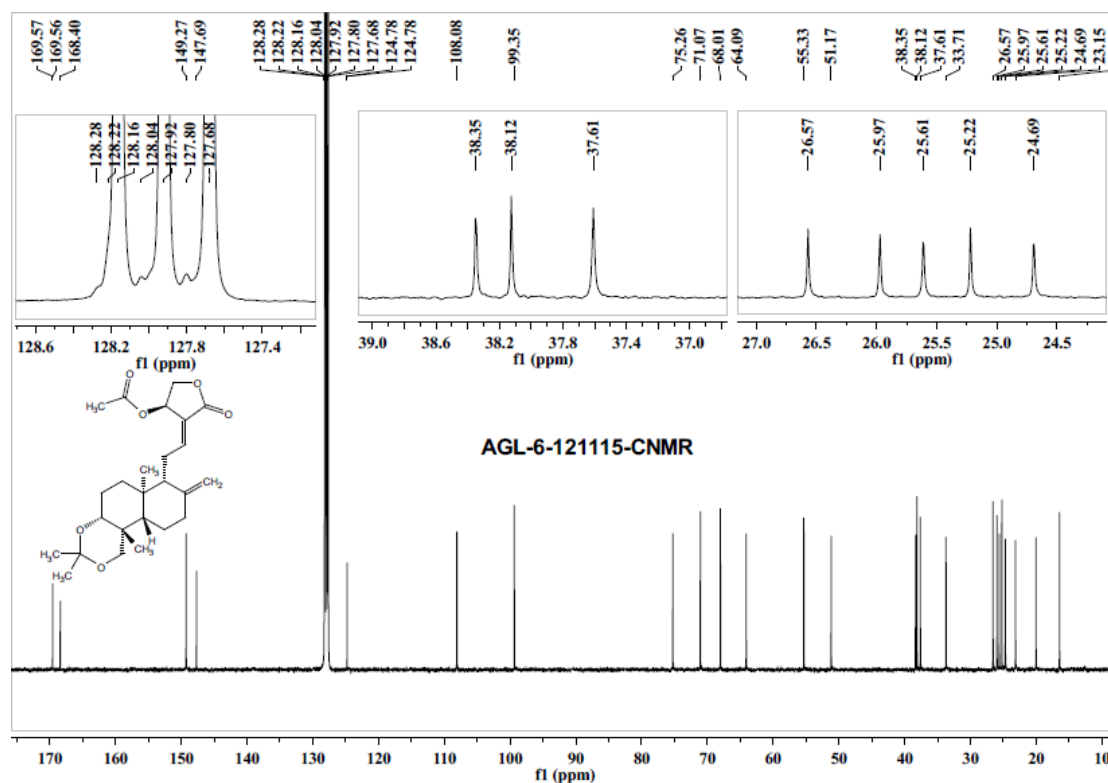
^{a)} See Scheme 2. ^{b)} calculated by Chem3D Ultra 8.0.

NMR spectra

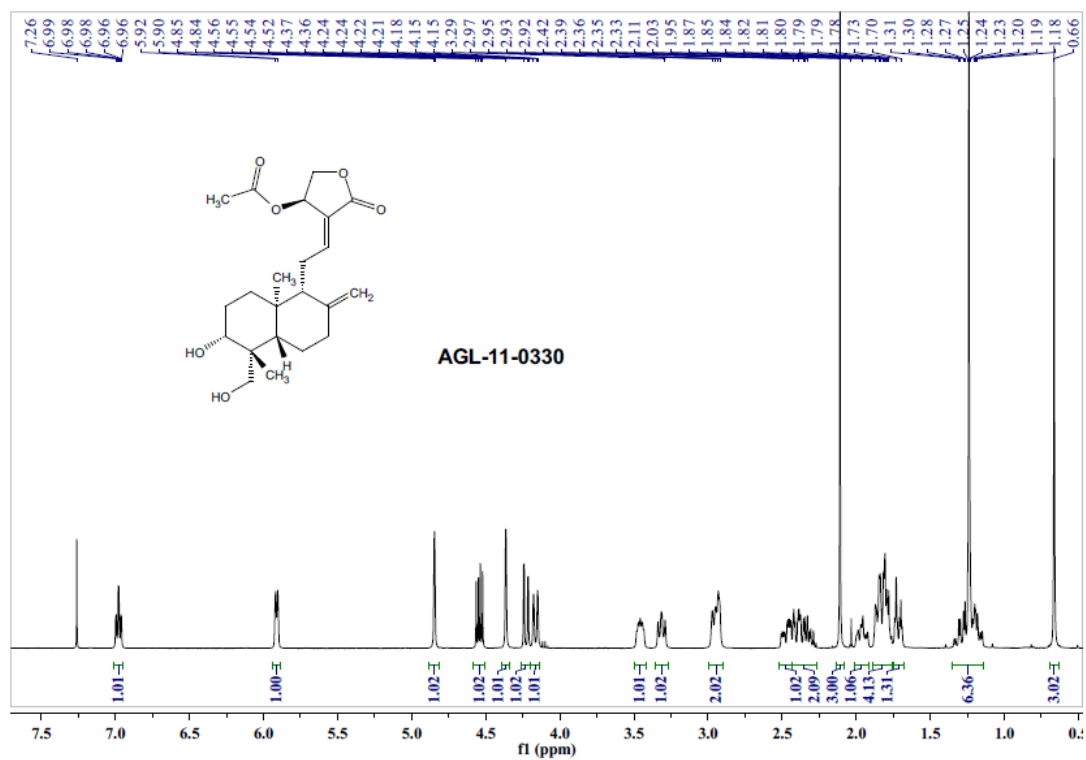
^1H NMR of Compound 6:



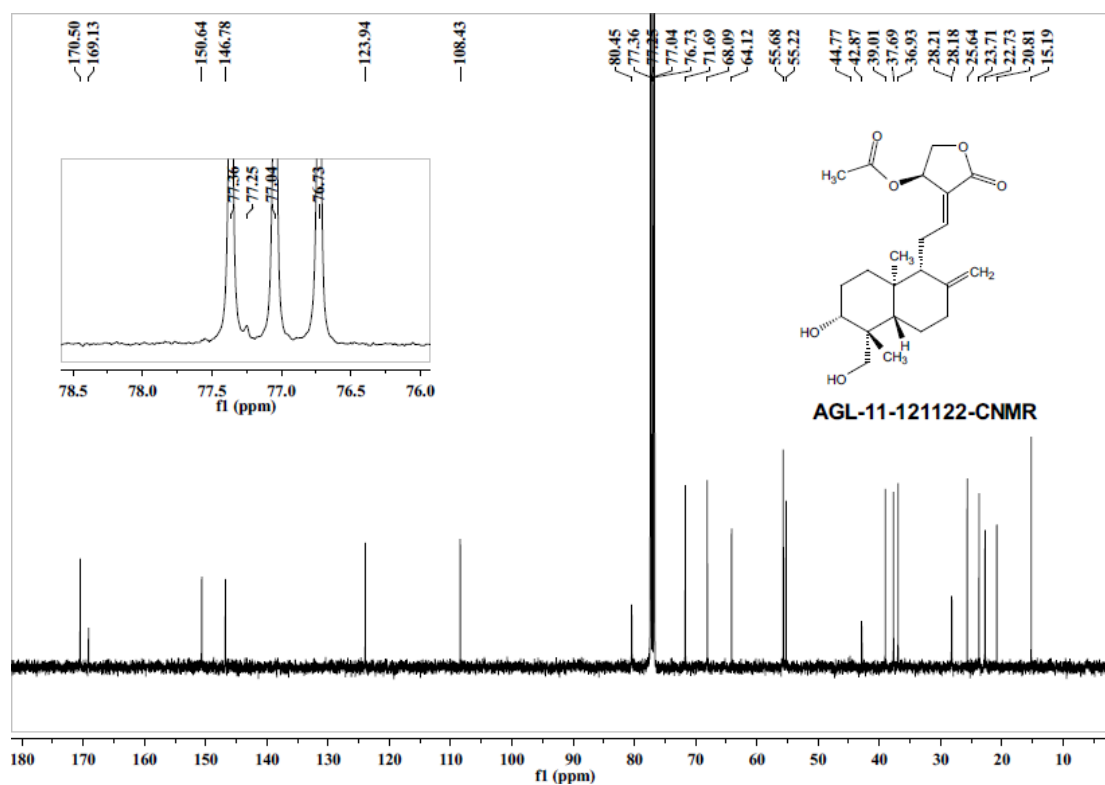
^{13}C NMR of Compound 6:



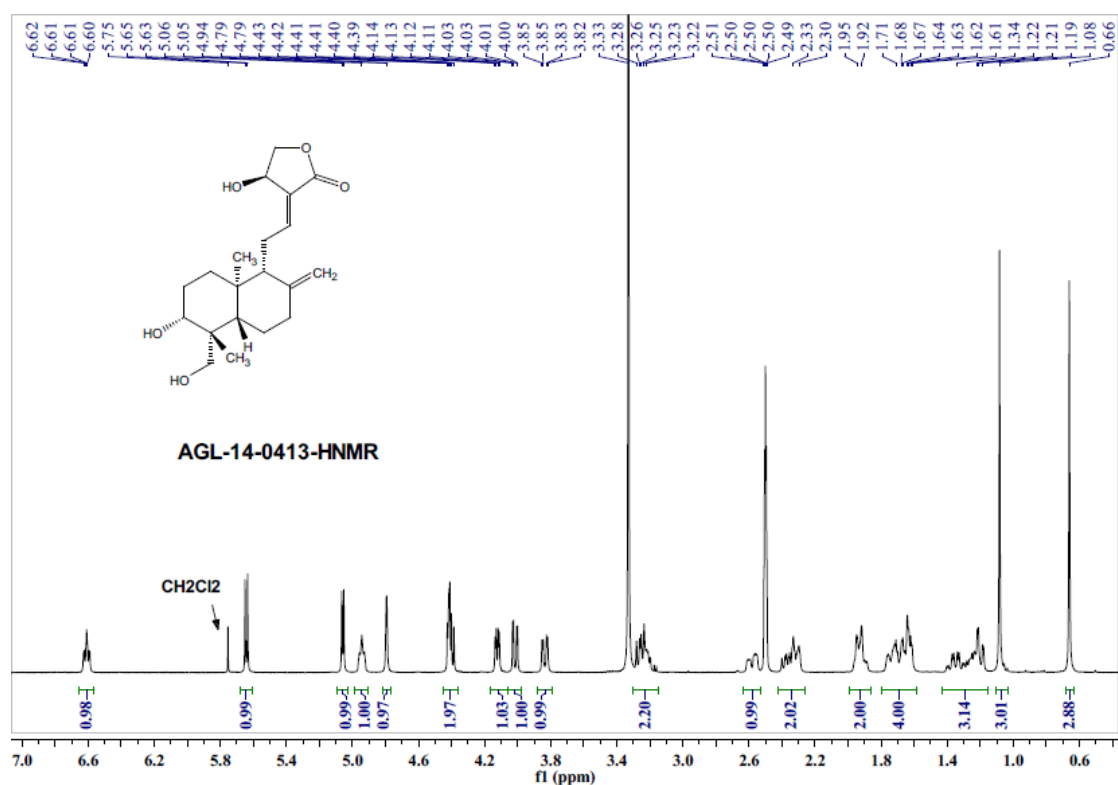
¹H NMR of **Compound 7**:



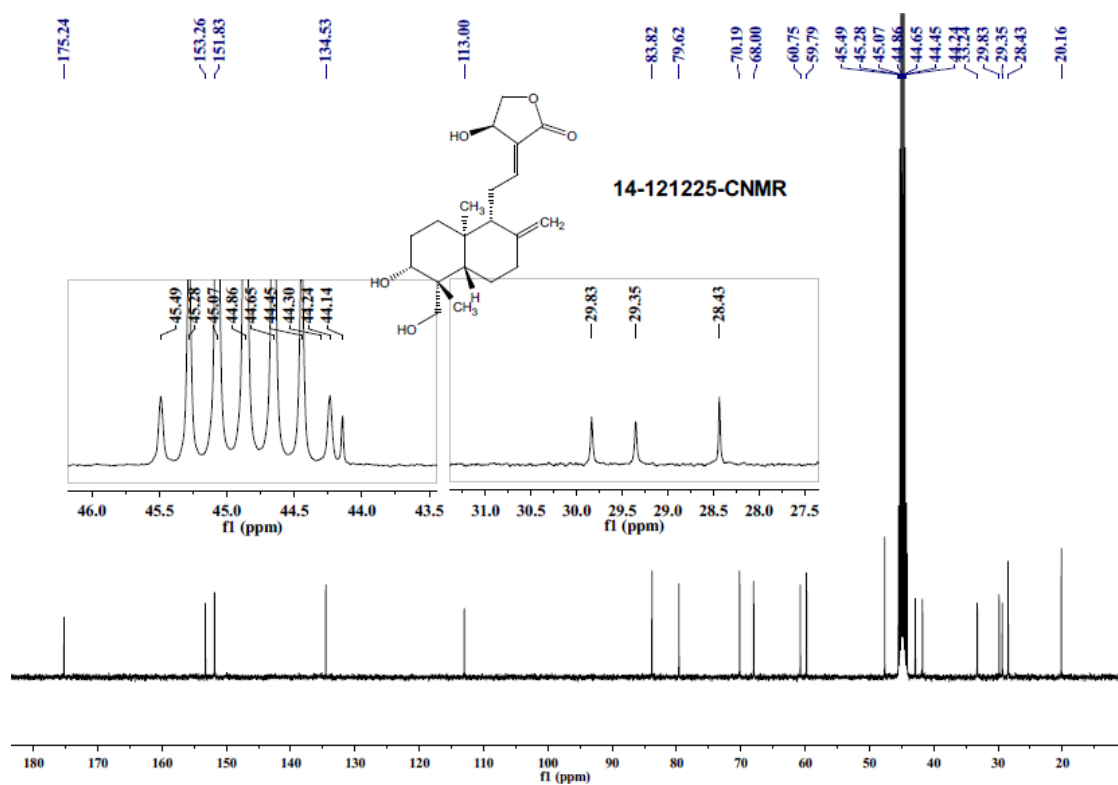
¹³C NMR of **Compound 7**:



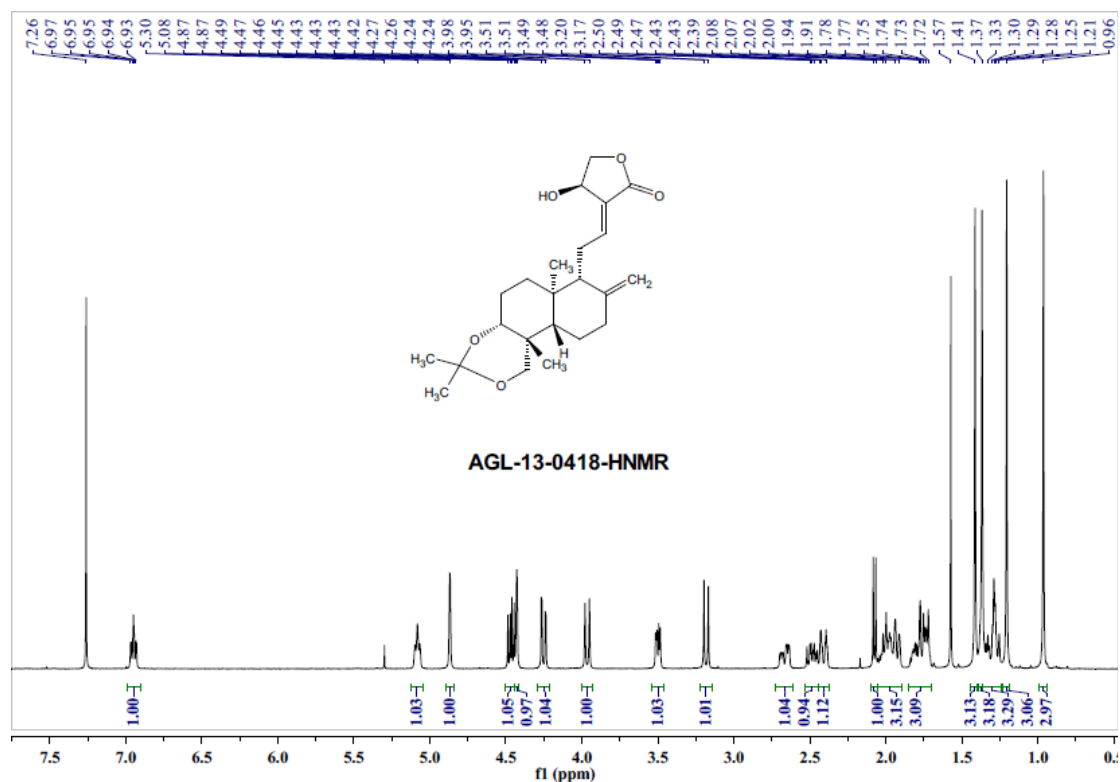
¹H NMR of **Compound 8**:



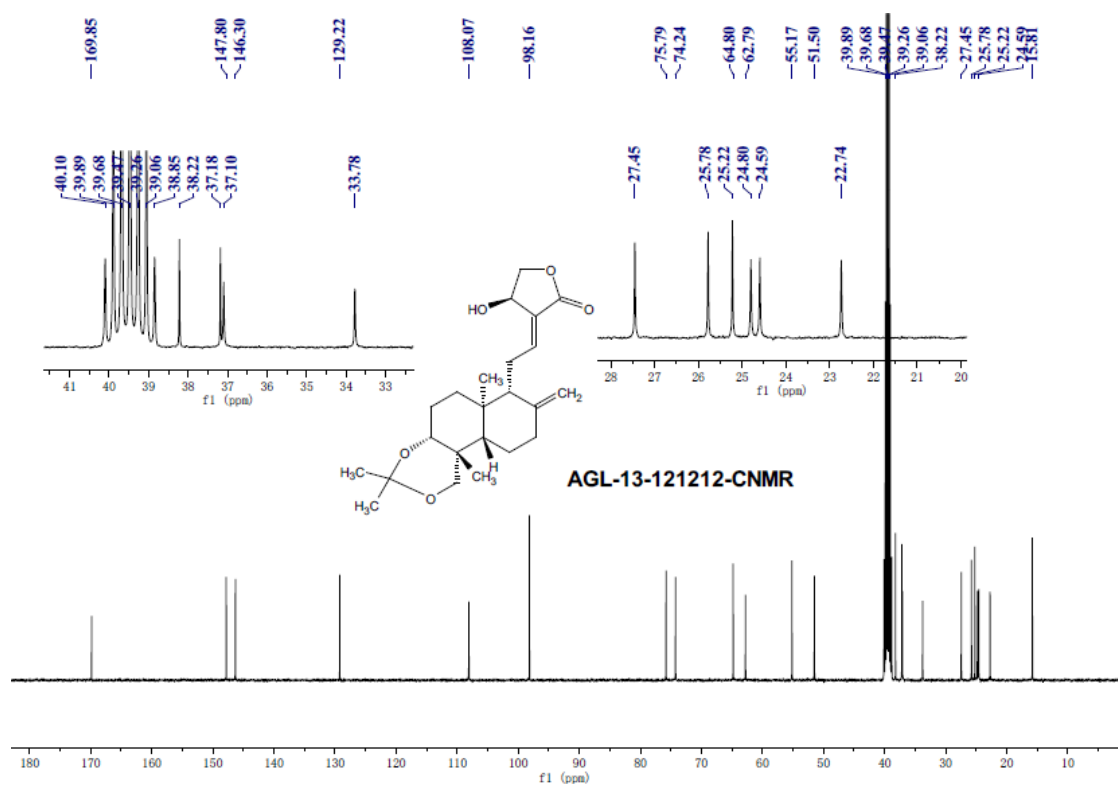
¹³C NMR of **Compound 8**:



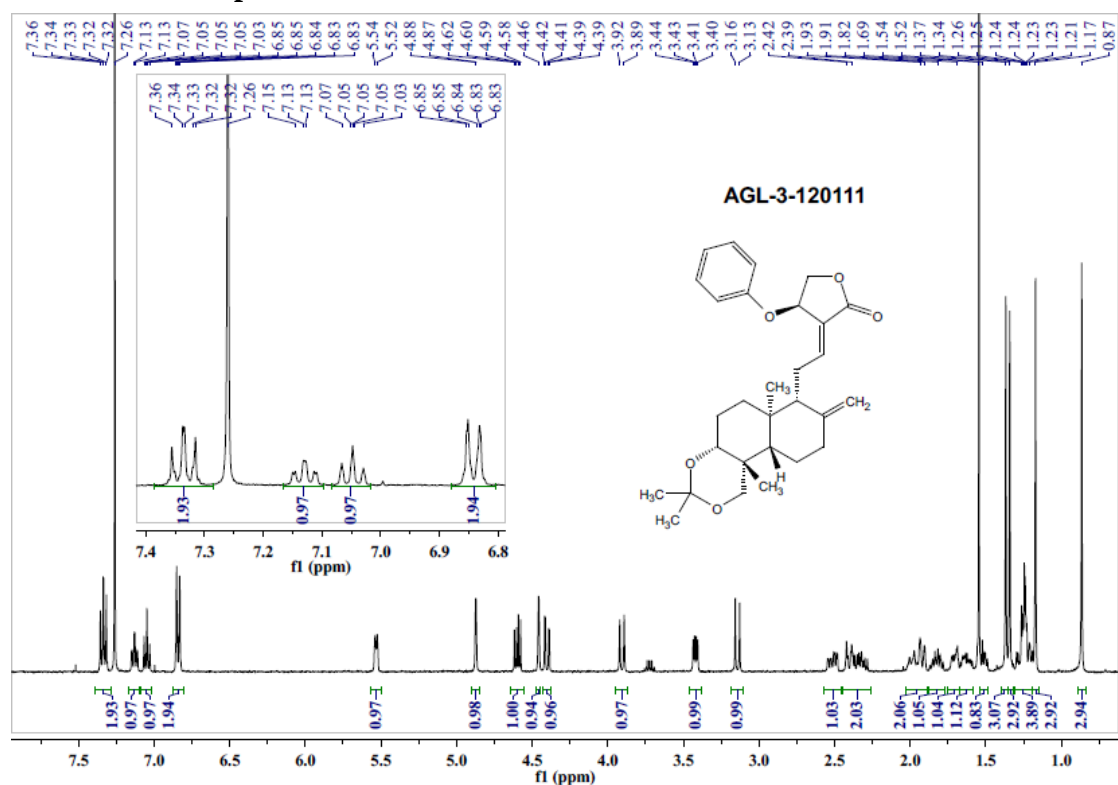
¹H NMR of **Compound 9**:



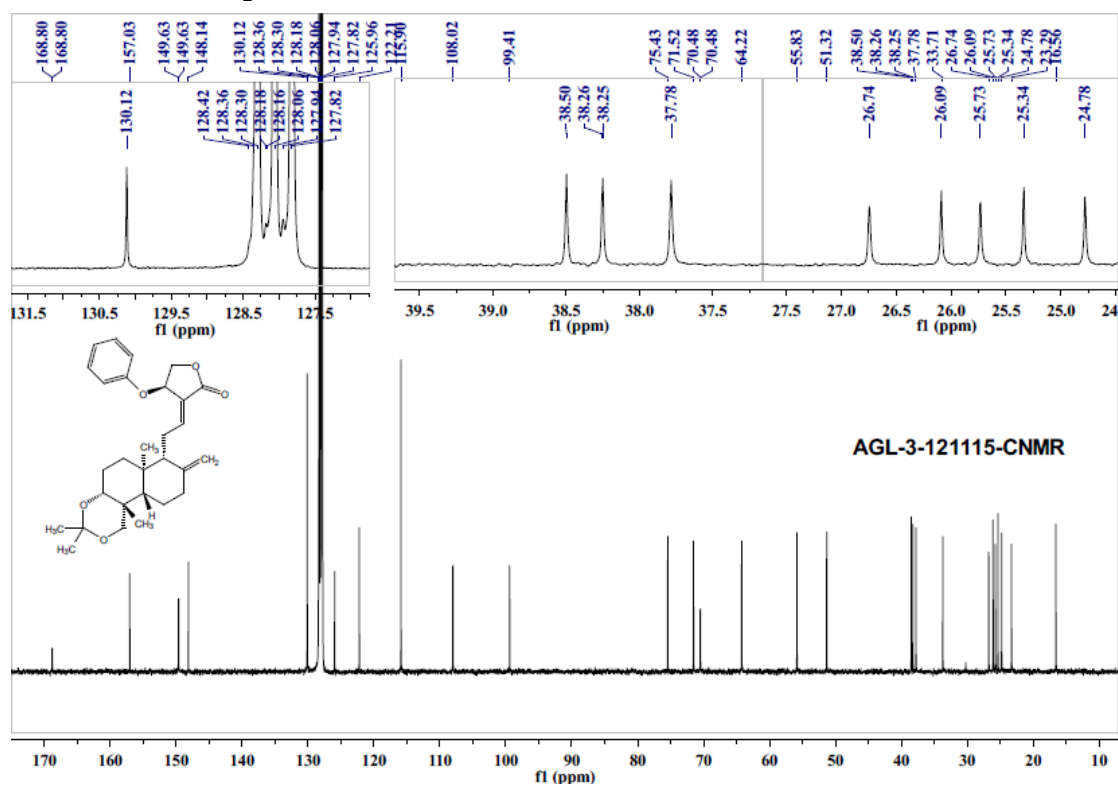
¹³C NMR of **Compound 9**:



¹H NMR of Compound 10a:



^{13}C NMR of Compound 10a:



AGL-4-120106

Chemical structure of AGL-4-120106 is shown above the spectrum. The structure is a complex polycyclic molecule with a steroid-like core, a methoxy group, a methyl group, and a side chain containing a double bond and a nitro group.

¹H NMR spectrum (CDCl₃) of AGL-4-120106. The x-axis represents the chemical shift in ppm, ranging from 0.5 to 8.5. The spectrum shows several peaks, with integration values provided below the peaks.

Chemical shift (ppm): 8.28, 8.27, 8.26, 7.26, 7.19, 6.94, 6.93, 6.92, 6.91, 5.66, 5.65, 4.90, 4.89, 4.89, 4.89, 4.69, 4.68, 4.66, 4.65, 4.45, 4.45, 4.45, 4.38, 4.38, 4.36, 4.36, 4.35, 4.35, 3.87, 3.87, 3.46, 3.45, 3.44, 3.43, 3.15, 3.12, 2.44, 2.40, 2.37, 2.04, 1.98, 1.93, 1.80, 1.79, 1.70, 1.56, 1.56, 1.52, 1.50, 1.35, 1.33, 1.28, 1.27, 1.26, 1.25, 1.23, 1.22, 1.16, 0.89.

Integration values (from left to right): 1.97, 1.01, 2.01, 1.00, 0.99, 1.01, 0.99, 1.01, 1.00, 1.00, 1.00, 1.02, 2.02, 2.02, 1.05, 0.97, 1.07, 0.94, 3.14, 3.16, 3.47, 3.01.

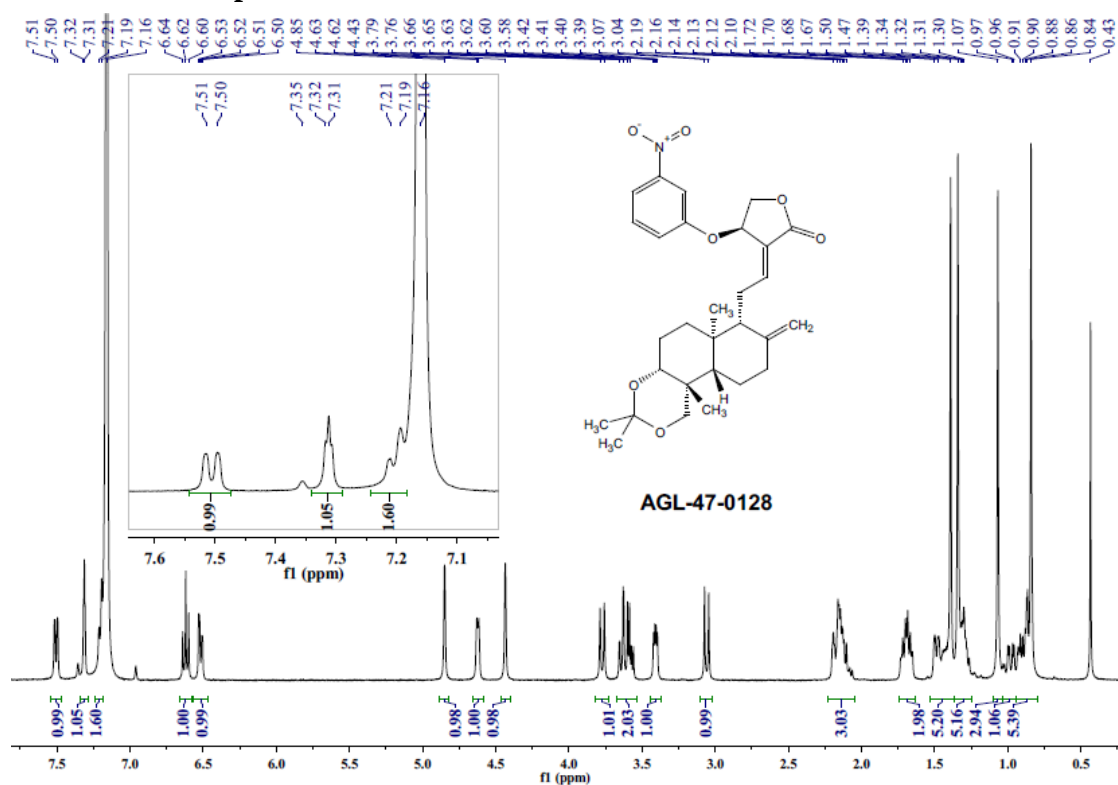
Chemical structure of AGL-4-1105 is shown. The structure is a complex polycyclic molecule with a p-nitrophenyl group and a 4,5-dimethyl-1,3-dioxolane ring.

AGL-4-1105-CNMR

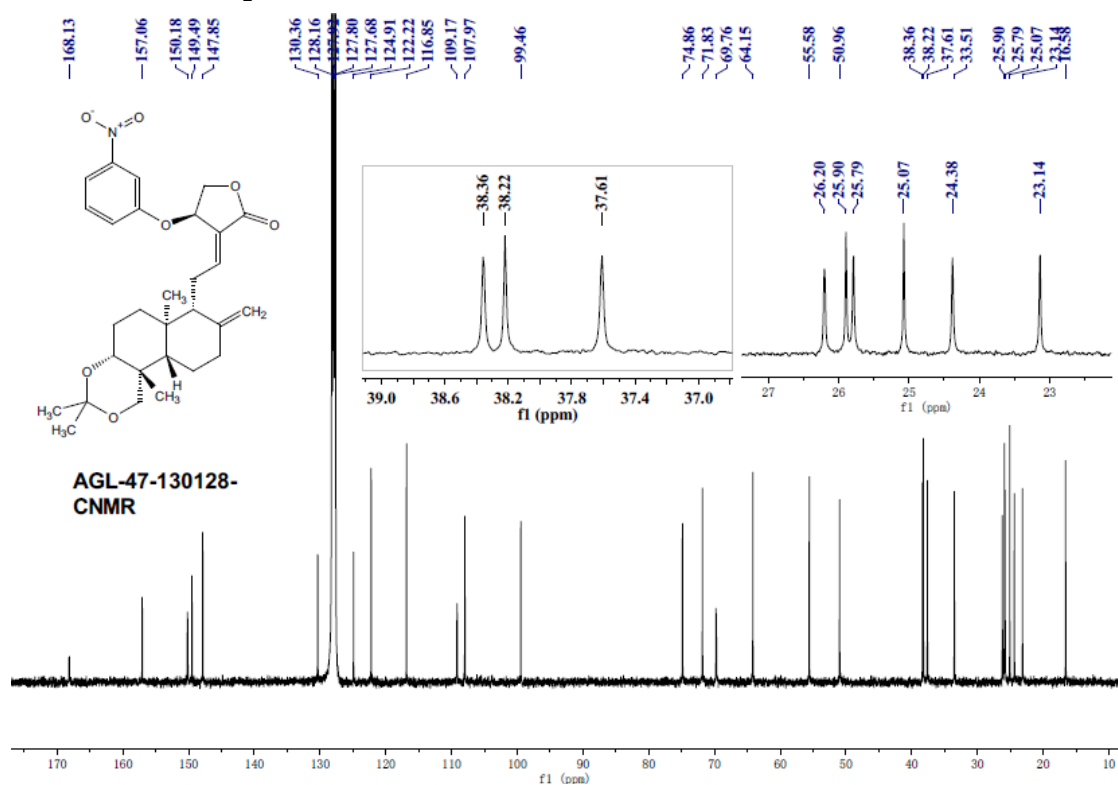
13C NMR peaks (ppm):

- 168.68, 161.28, 151.98, 147.27, 142.53, 126.35, 123.93, 115.16, 108.26, 99.37, 77.36, 77.36, 77.24, 77.04, 77.04, 76.78, 76.73, 76.72, 75.42, 71.78, 70.26, 64.05, 55.82, 51.66, 38.50, 38.10, 37.58, 26.47, 26.01, 25.94, 25.10, 24.43, 23.17.

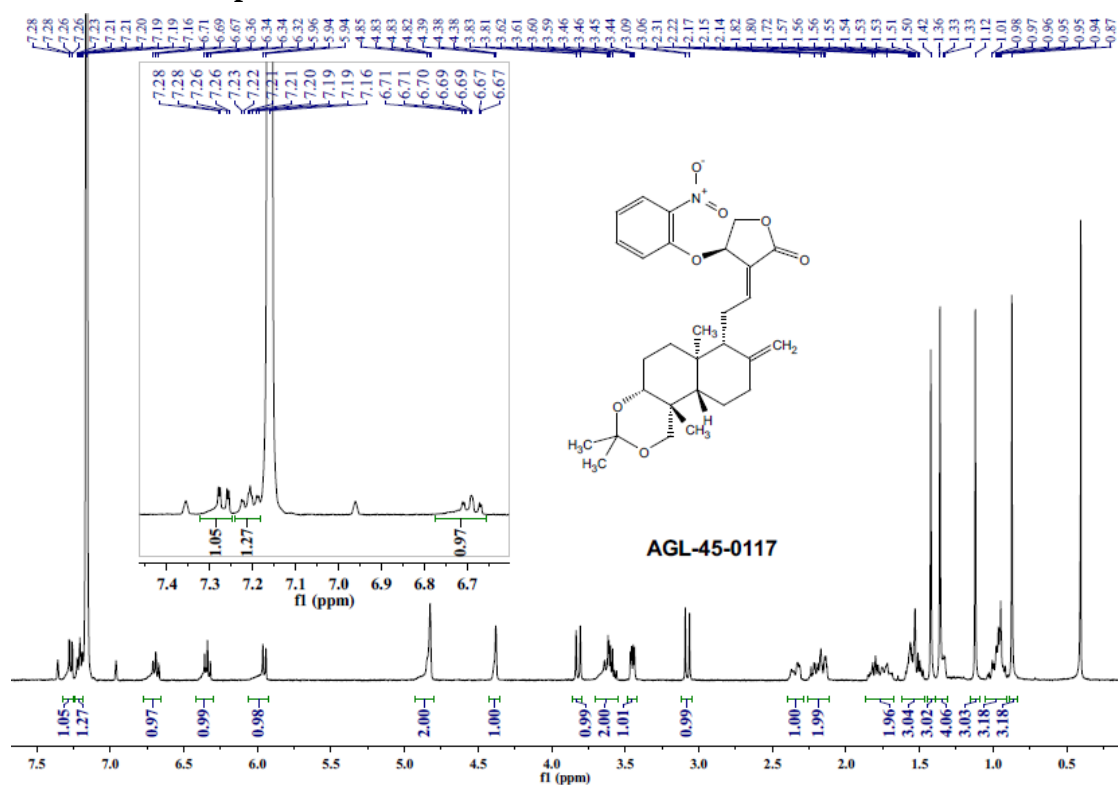
¹H NMR of Compound 10c:



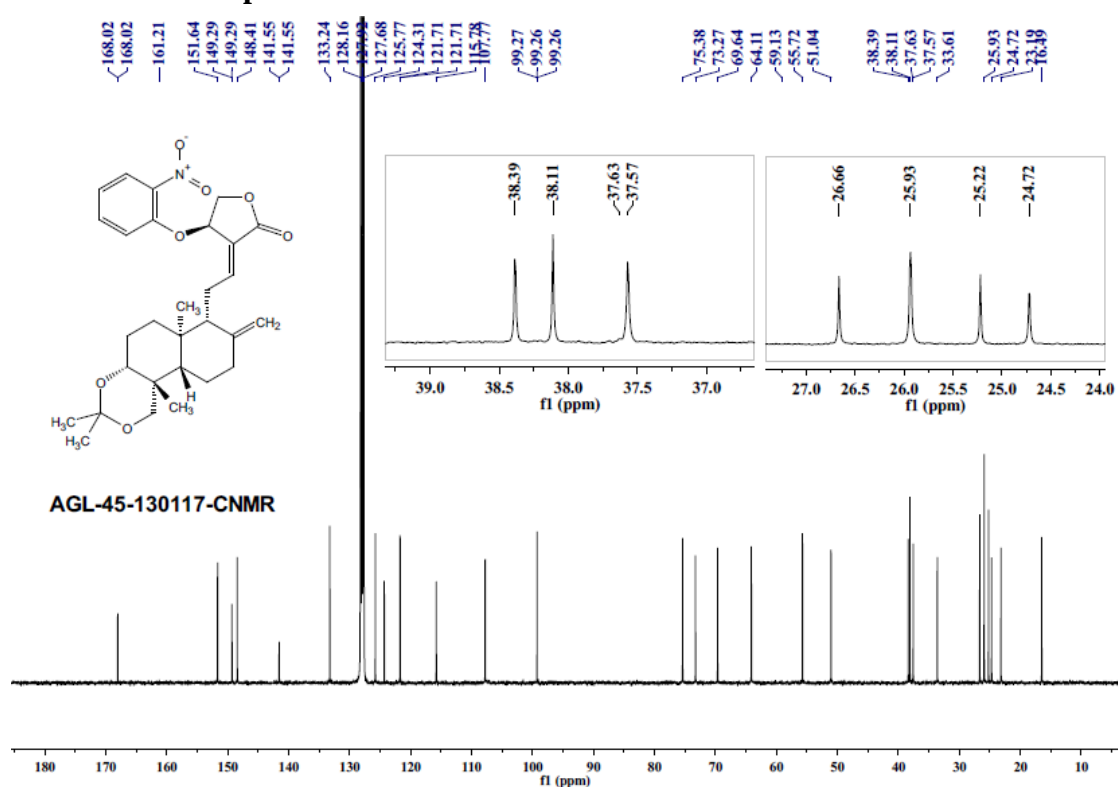
¹³C NMR of Compound 10c:



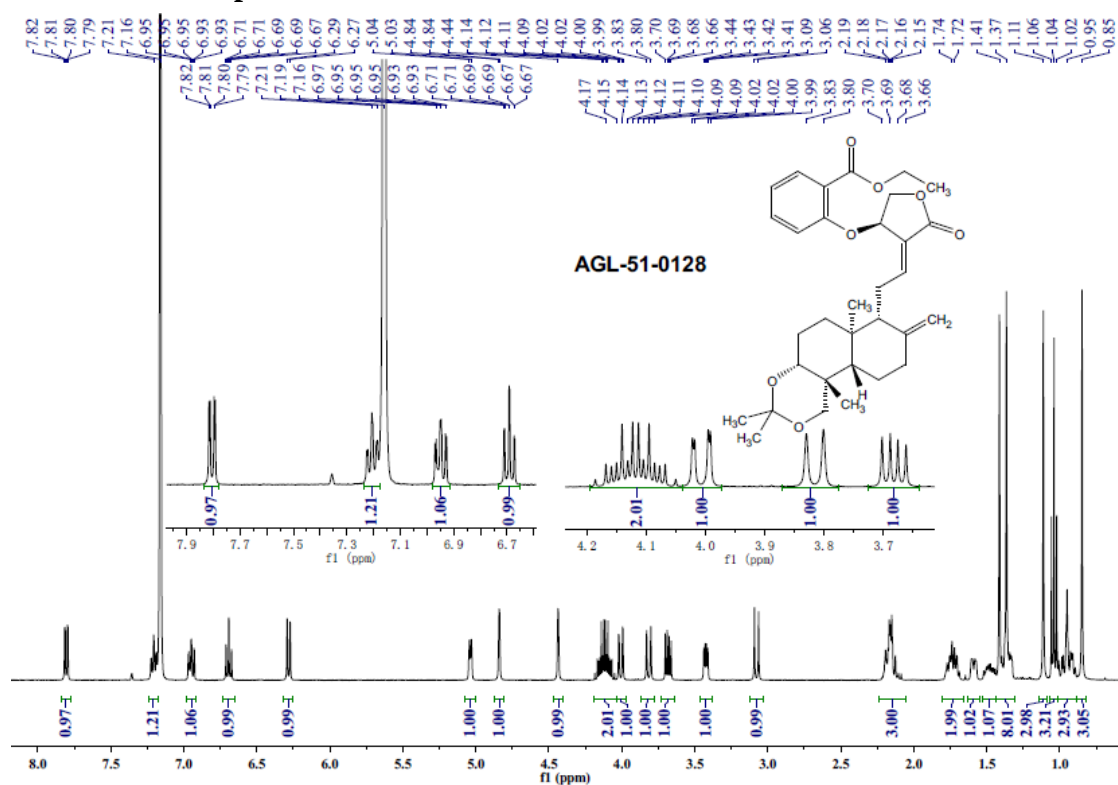
¹H NMR of Compound 10d:



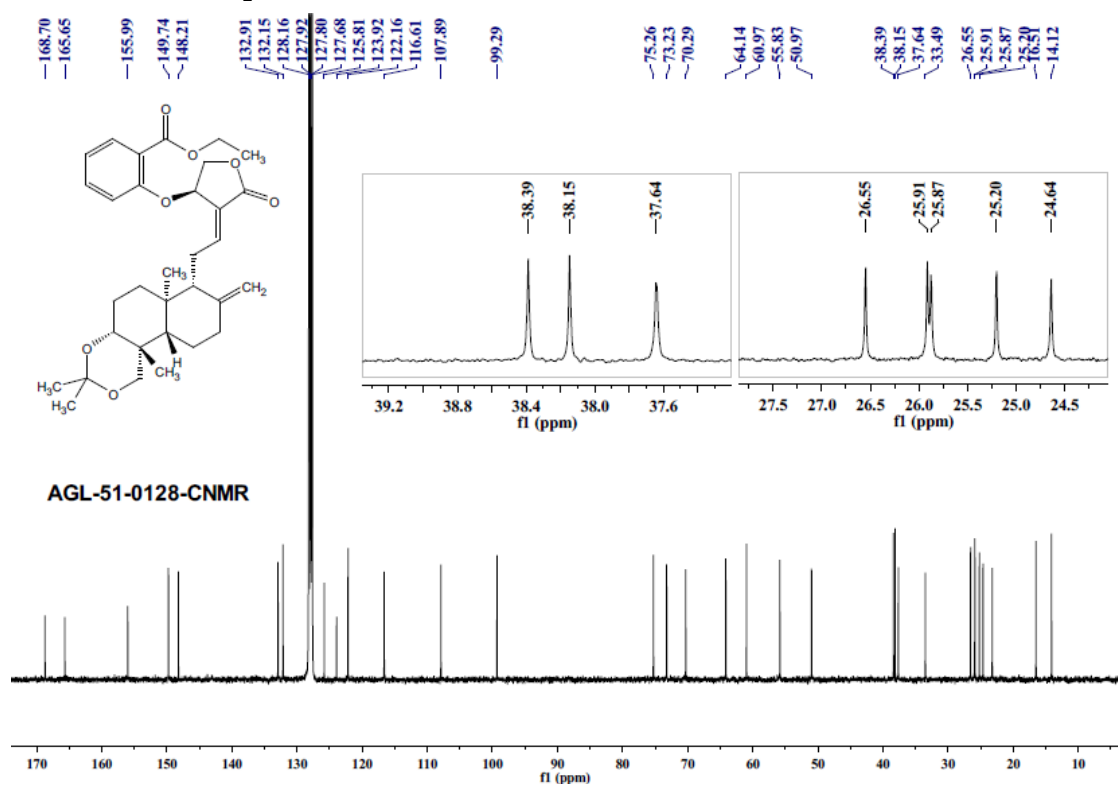
¹³C NMR of Compound 10d:



¹H NMR of Compound 10e:



¹³C NMR of Compound 10e:



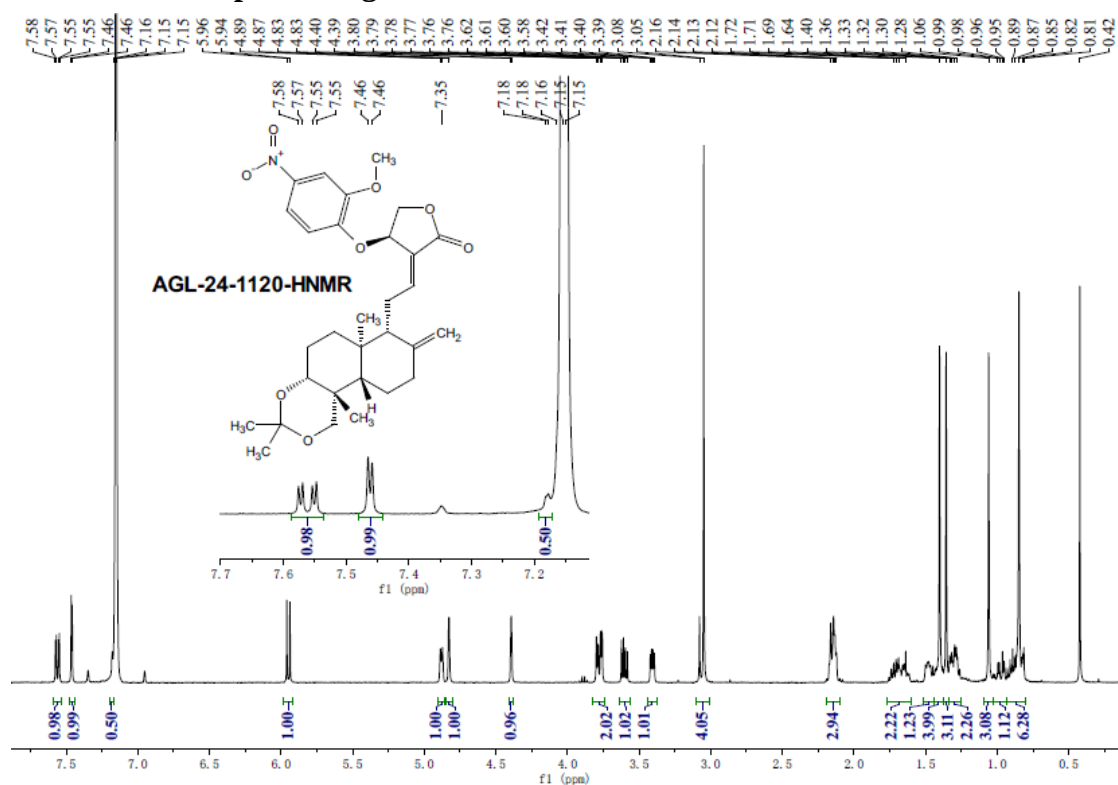
Chemical structure of compound 1 (AGL-61-0423-HNMR) is shown. The structure is a complex polycyclic molecule, likely a natural product or synthetic derivative, featuring a benzodioxane system, a cyclohexene ring, and a furanone moiety.

The ¹H NMR spectrum (CDCl₃) shows peaks corresponding to the structure. The inset shows the aromatic region (6.4-7.2 ppm) with peaks at 7.15, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0.82, 0.81, 0.80, 0.79, 0.78, 0.77, 0.76, 0.75, 0.74, 0.73, 0.72, 0.71, 0.7

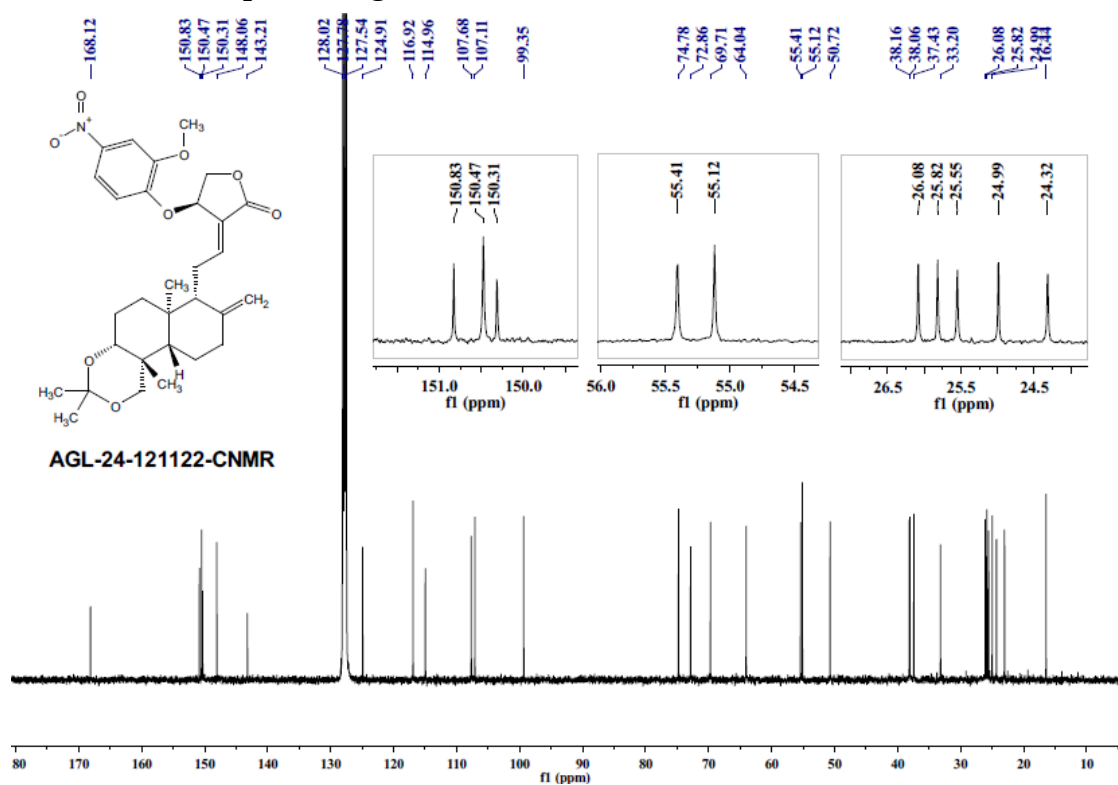
AGL-61-0423-CNMR

Chemical structure of AGL-61-0423 is shown. The structure is a complex polycyclic molecule with a benzene ring, a furanone ring, and a decalin-like core. The peaks are labeled with their chemical shifts in ppm: 169.08, 151.78, 149.42, 148.27, 145.92, 128.15, 128.03, 127.91, 127.67, 126.39, 124.00, 121.11, 119.18, 107.85, 99.30, 75.39, 73.44, 70.36, 64.14, 55.72, 55.11, 51.10, 38.34, 38.12, 37.66, 26.57, 26.00, 25.64, 25.29, 24.74.

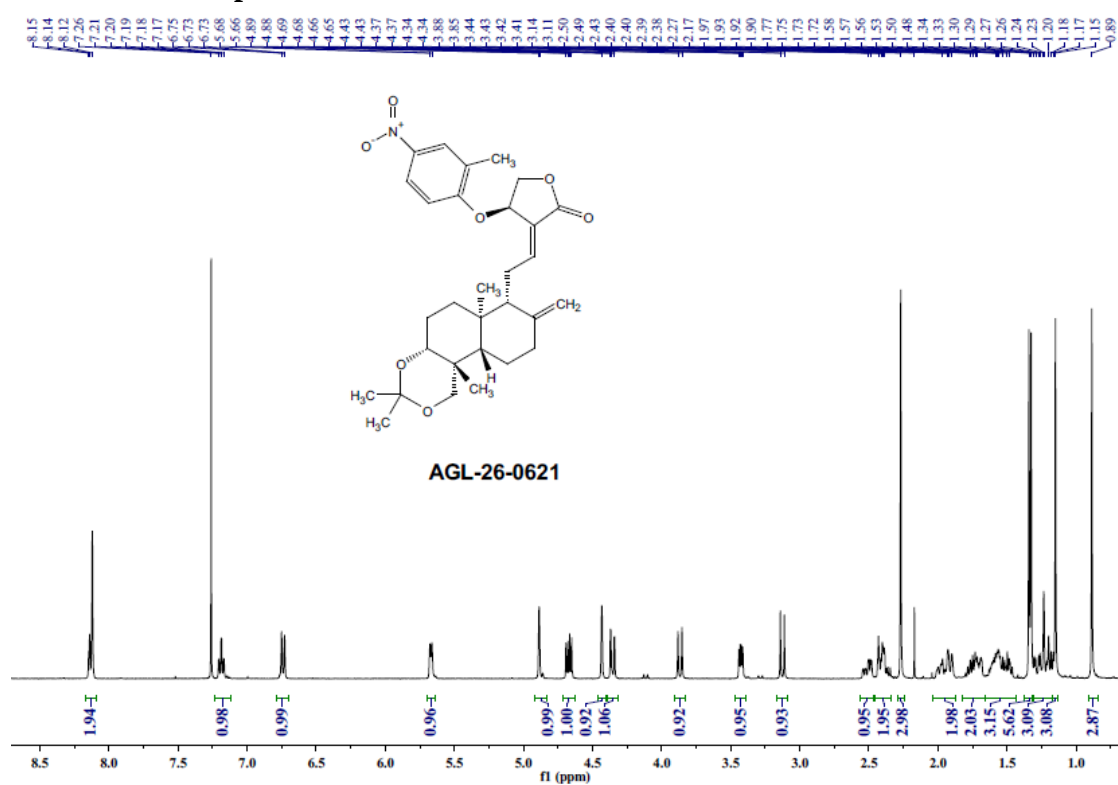
¹H NMR of Compound 10g:



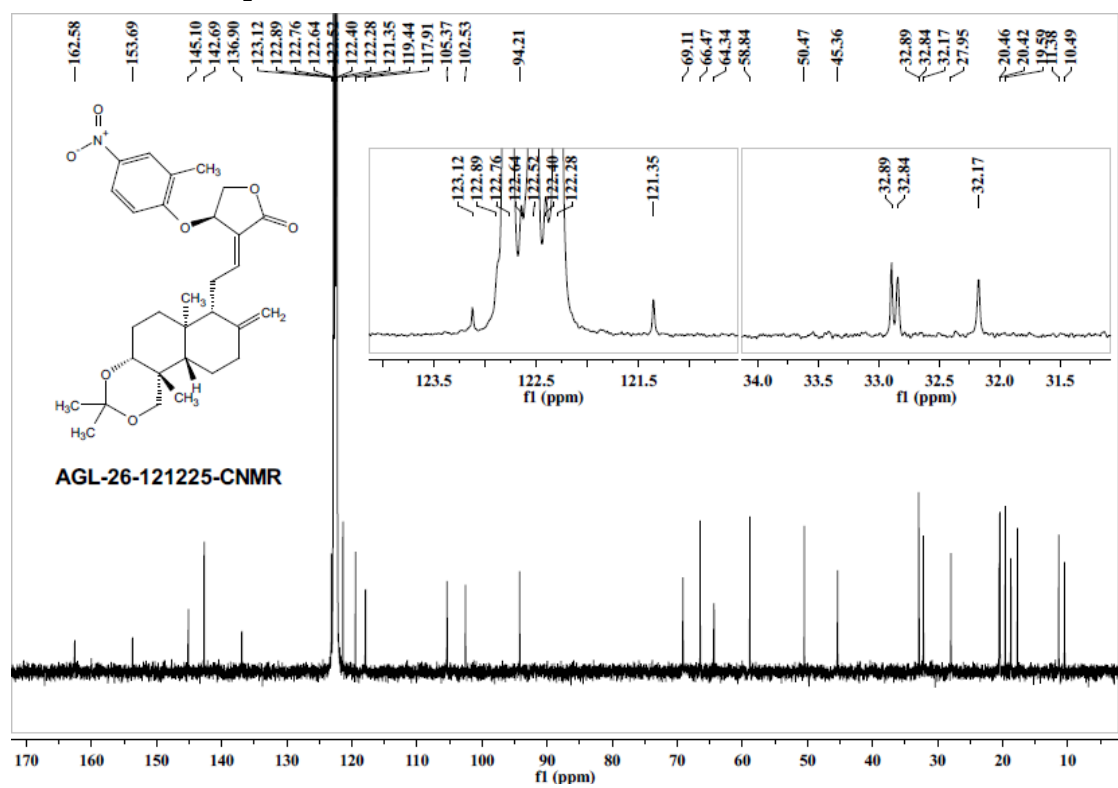
¹³C NMR of Compound 10g:



¹H NMR of Compound 10h:



¹³C NMR of Compound 10h:



AGS-13-0104-HNMR

Chemical structure of compound 104 is shown. The structure features a benzene ring substituted with a nitro group (NO₂) and a furanose ring. The furanose ring is connected to a bicyclic system via a methylene group. The bicyclic system includes a cyclohexane ring with a methyl group and a cyclopropane ring. The spectrum shows peaks corresponding to these structures, with integration values provided for several peaks.

AGL-18-0425

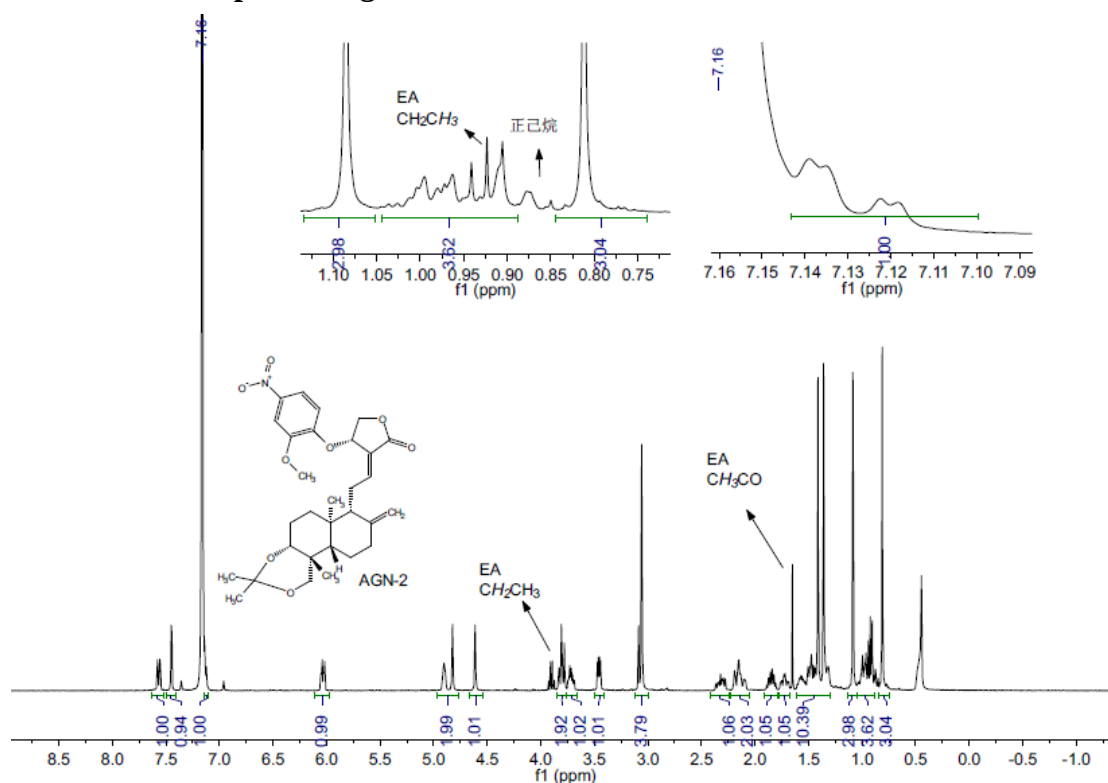
Chemical structure of AGL-18-0425 is shown above the spectrum. The structure is a complex molecule featuring a bicyclic core with a methoxy group, a methyl group, and a side chain containing a double bond and a nitro group.

¹H NMR spectrum (CDCl₃) data:

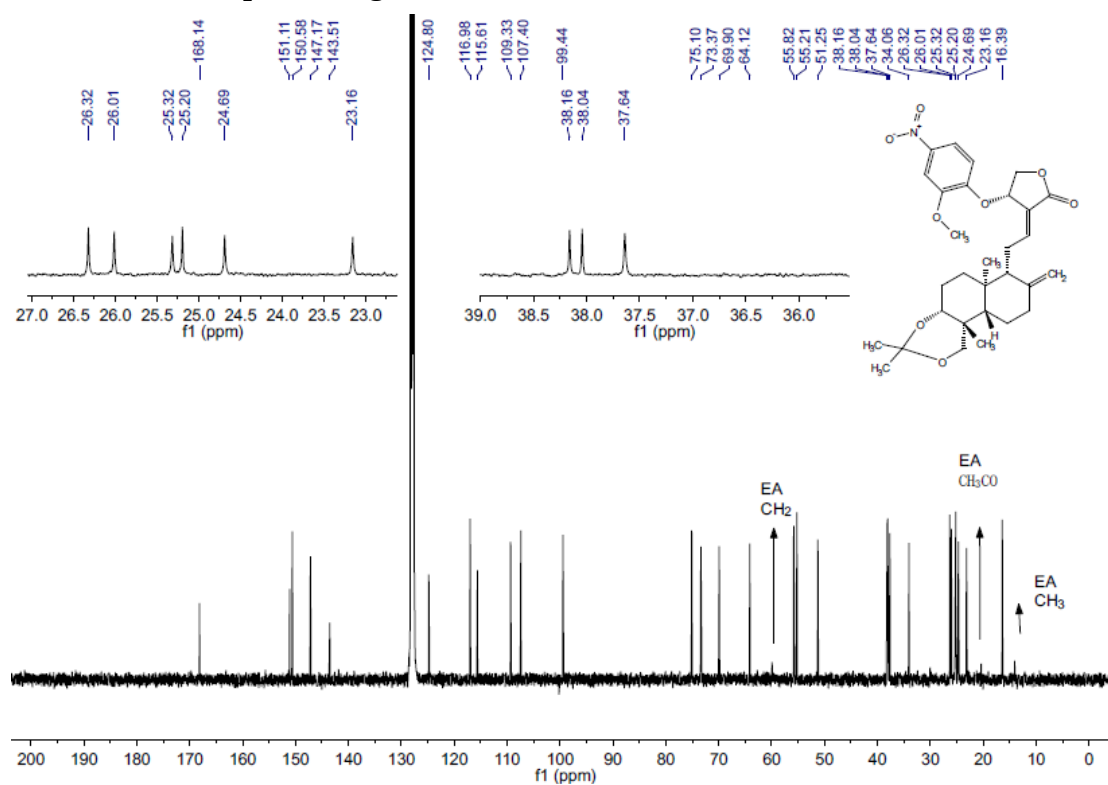
Chemical Shift (ppm)	Integration
7.78, 7.77, 7.76, 7.75, 7.74, 7.73, 7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.	

AGL-18-0425-CNMR

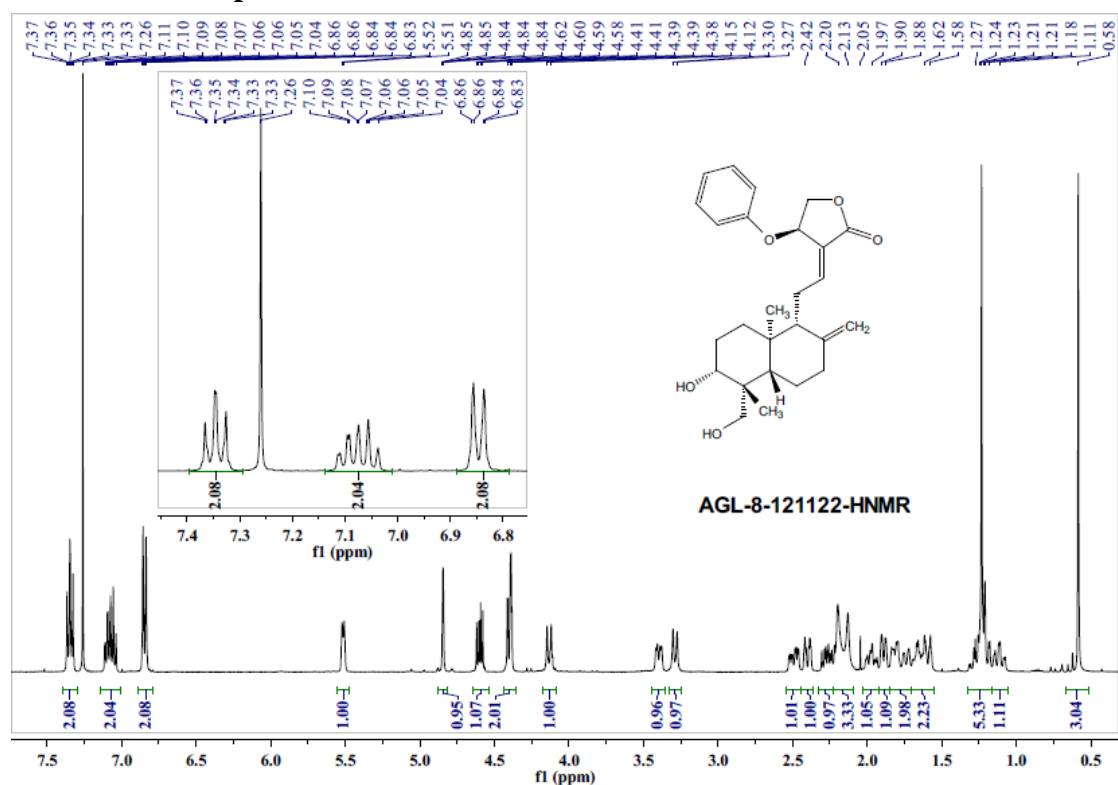
¹H NMR of **Compound 11g**:



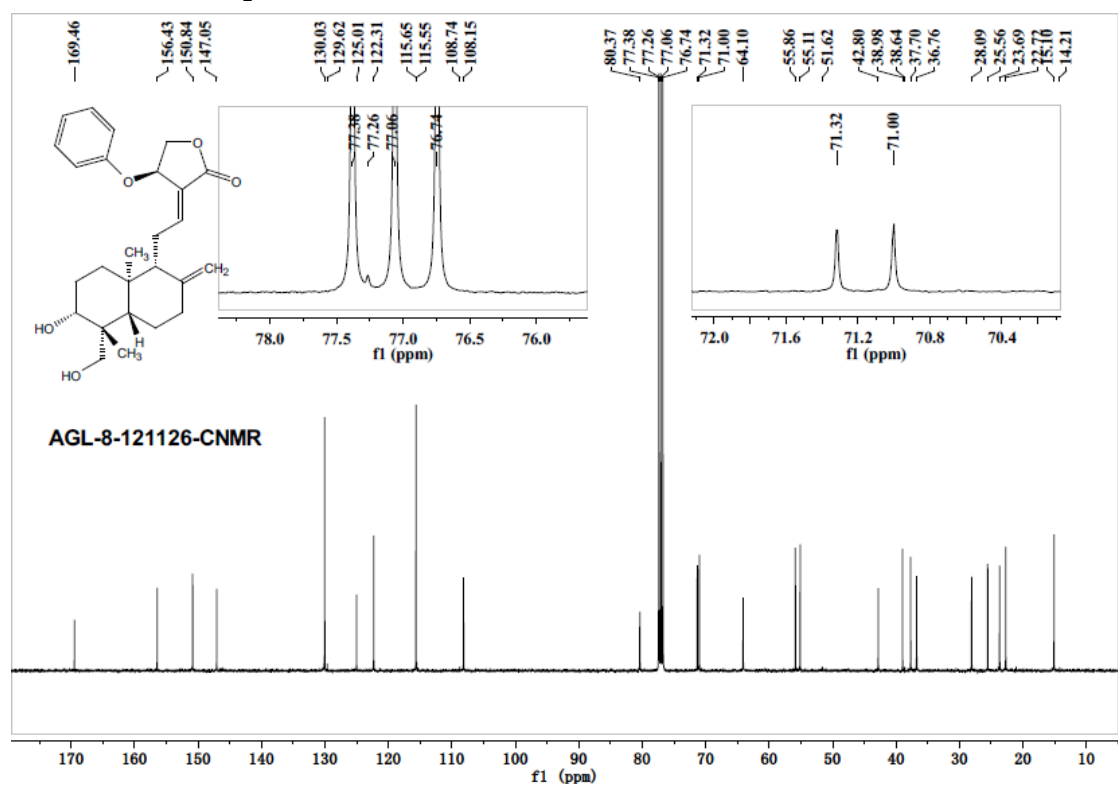
¹³C NMR of **Compound 11g**:



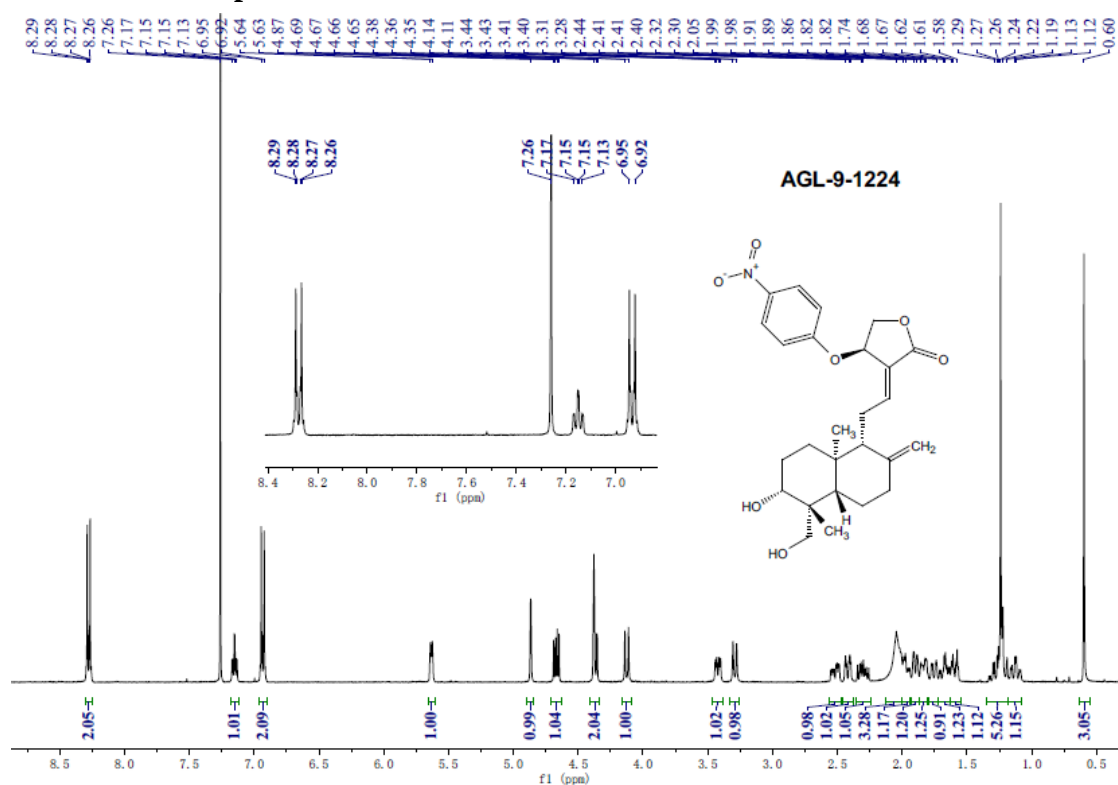
¹H NMR of Compound 12a:



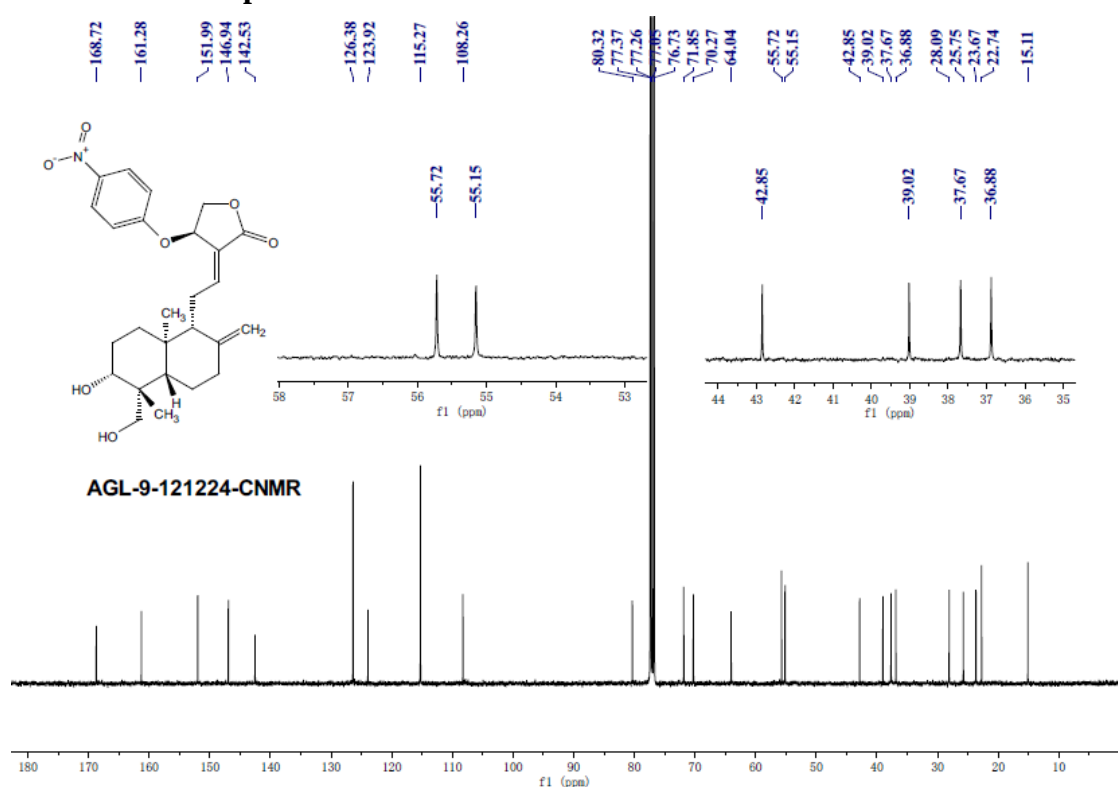
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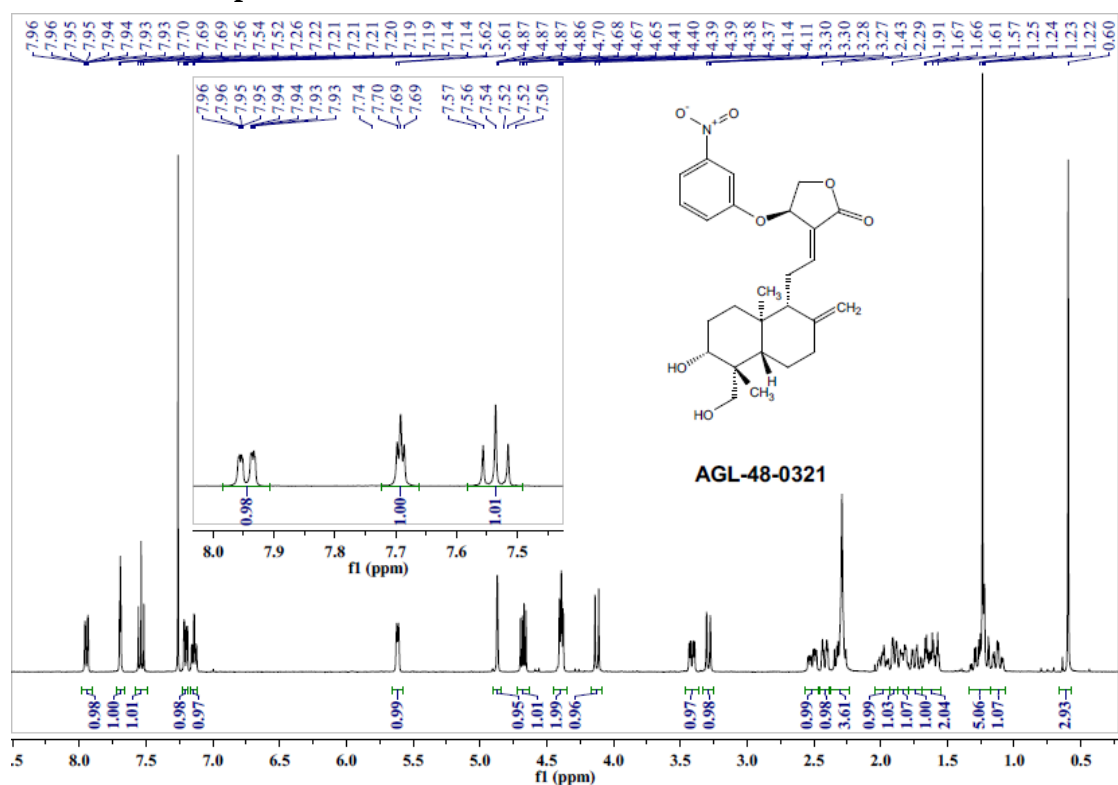
¹H NMR of Compound 12b:



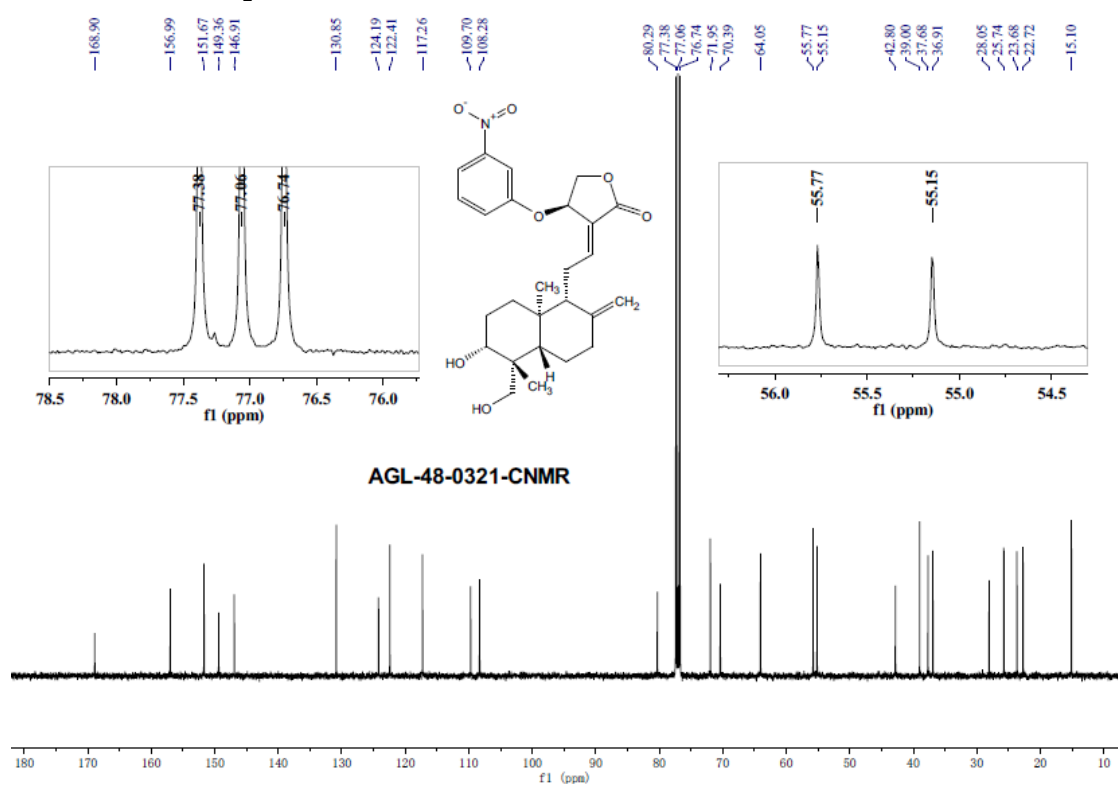
¹³C NMR of Compound 12b:



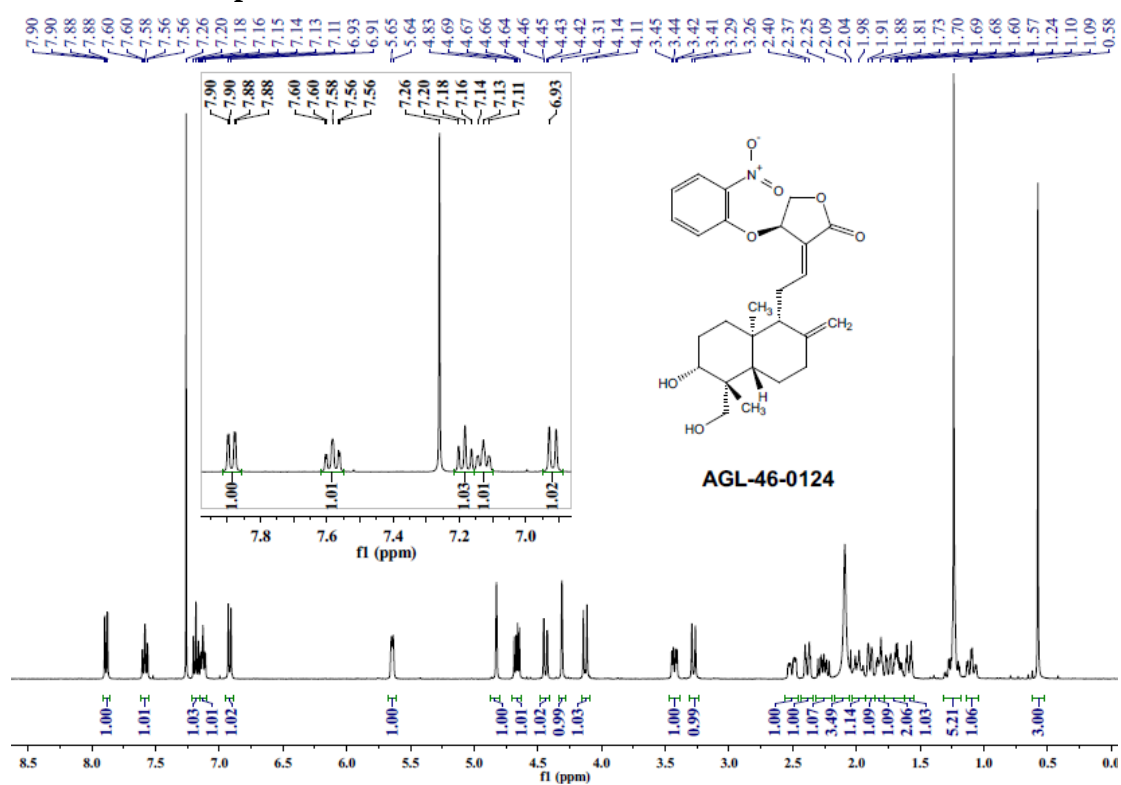
¹H NMR of **Compound 12c**:



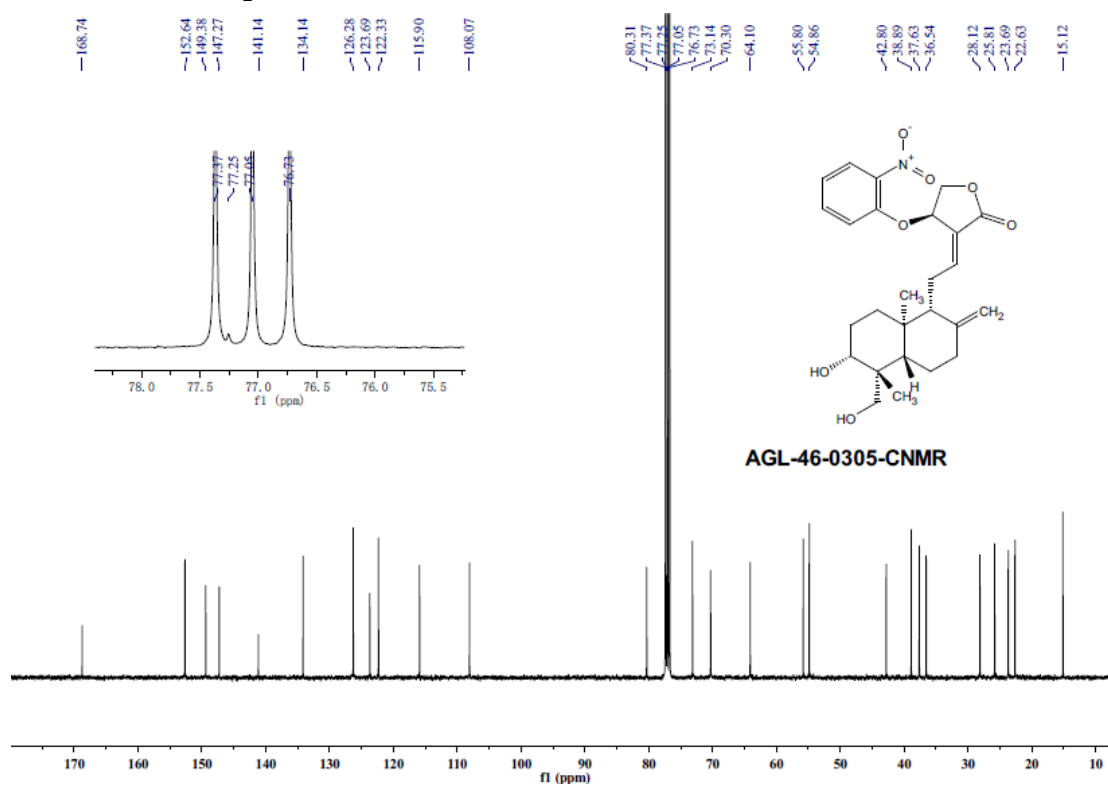
¹³C NMR of **Compound 12c**:



¹H NMR of **Compound 12d**:



¹³C NMR of **Compound 12d**:

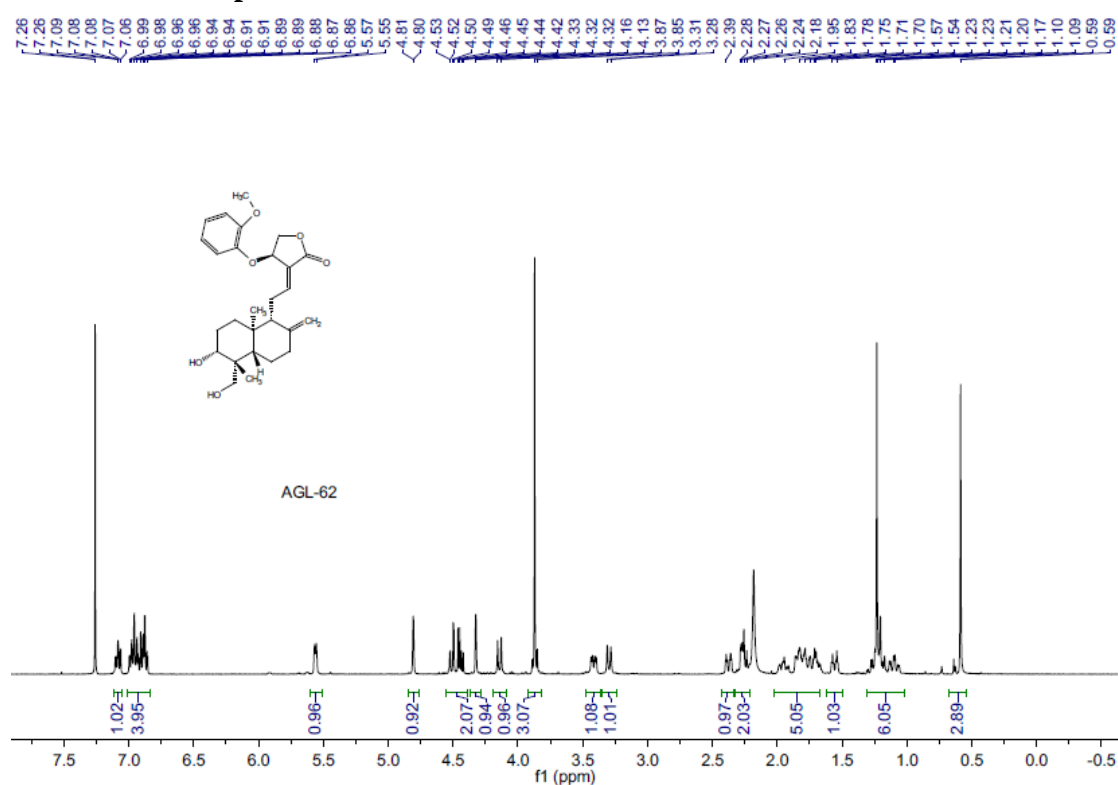


Chemical structure of compound 10 is shown. The ^1H NMR spectrum (400 MHz, CDCl_3) displays peaks corresponding to the structure, with chemical shifts and integrations provided for the aromatic and aliphatic regions.

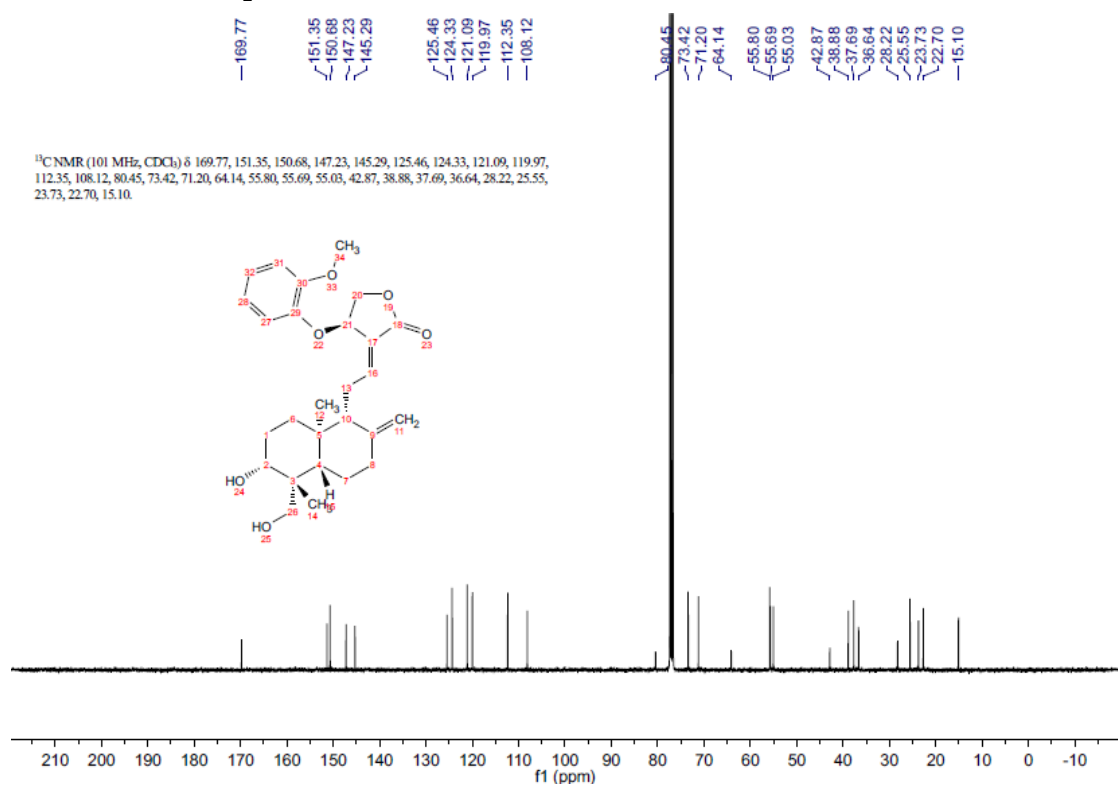
¹³C NMR spectra (B11-0228-CNMR) of compound 1. The chemical structure of compound 1 is shown above the spectra. The spectra are recorded in CDCl₃. The x-axis represents the chemical shift in ppm (f1), ranging from 180 to 10 for the top spectrum and 78.8 to 76.2 for the bottom spectrum. The top spectrum shows peaks at 169.45, 165.73, 155.78, 150.94, 147.11, 133.38, 132.26, 124.95, 123.22, 122.60, 117.01, and 108.19 ppm. The bottom spectrum shows peaks at 80.33, 77.36, 77.04, 76.73, 73.39, 70.98, 61.16, 55.76, 54.90, 42.81, 38.81, 37.63, 36.55, 28.12, 25.64, 23.68, 22.64, 15.07, and 14.29 ppm.

B11-0228-CNMR

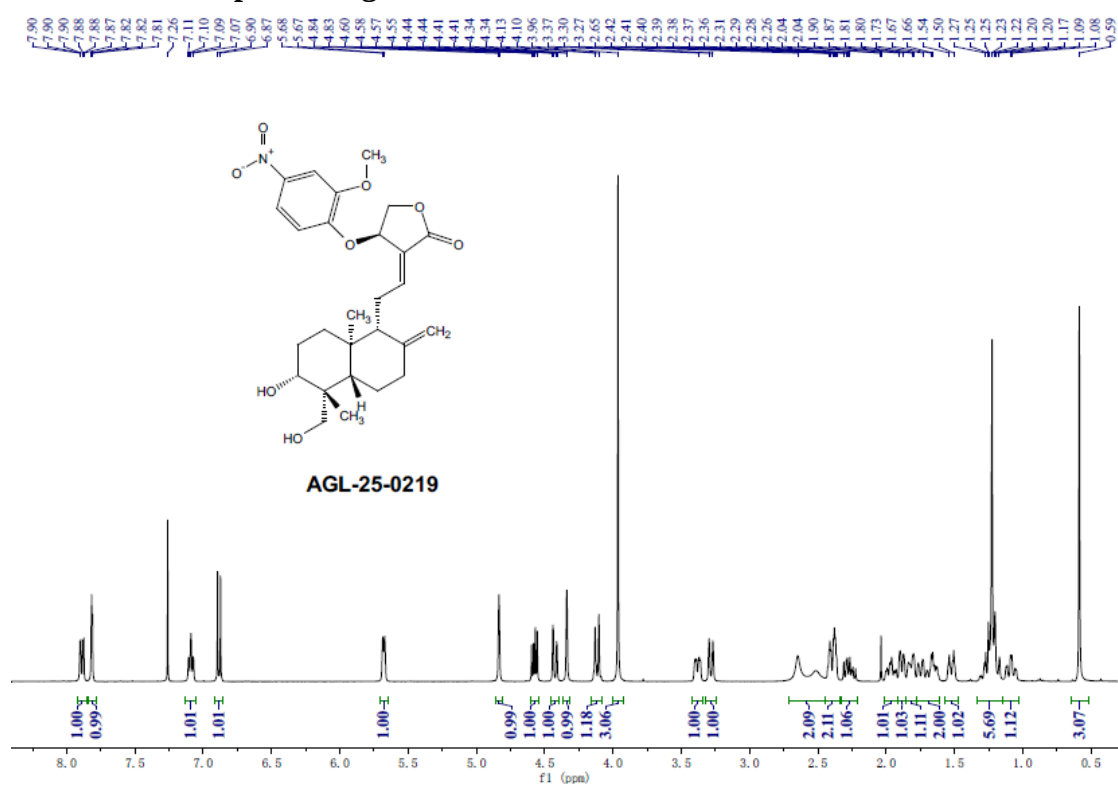
¹H NMR of Compound 12f:



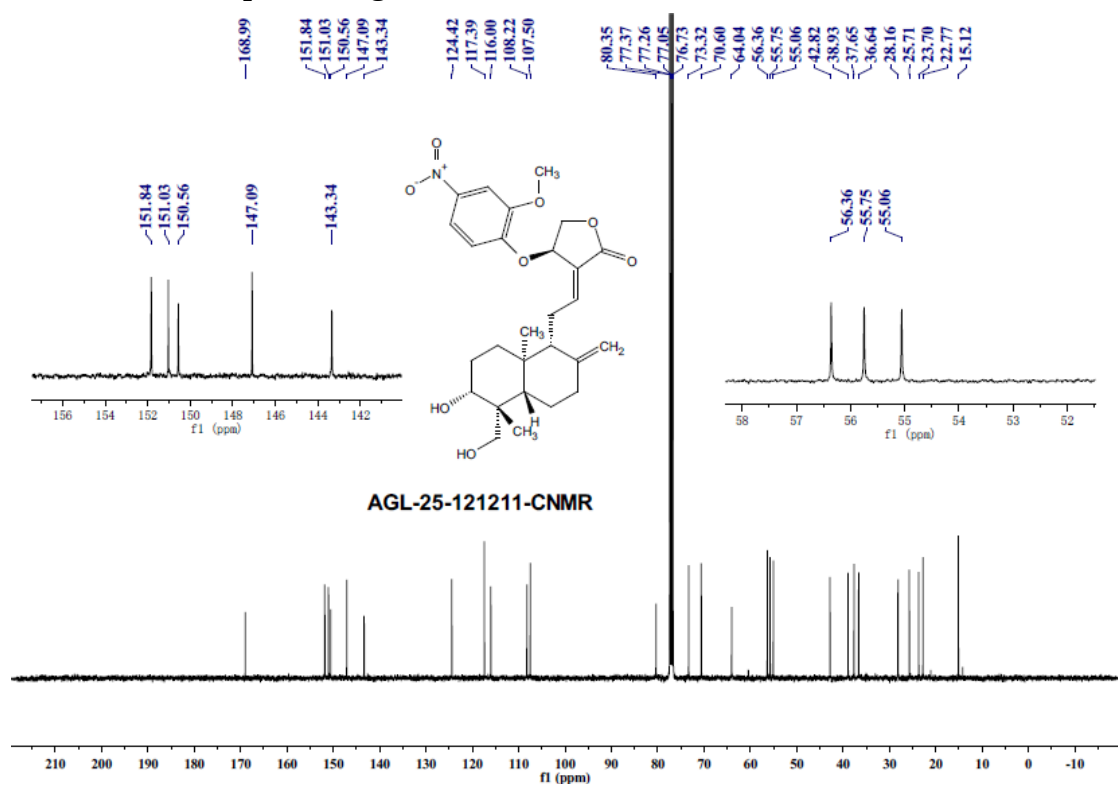
¹³C NMR of Compound 12f:



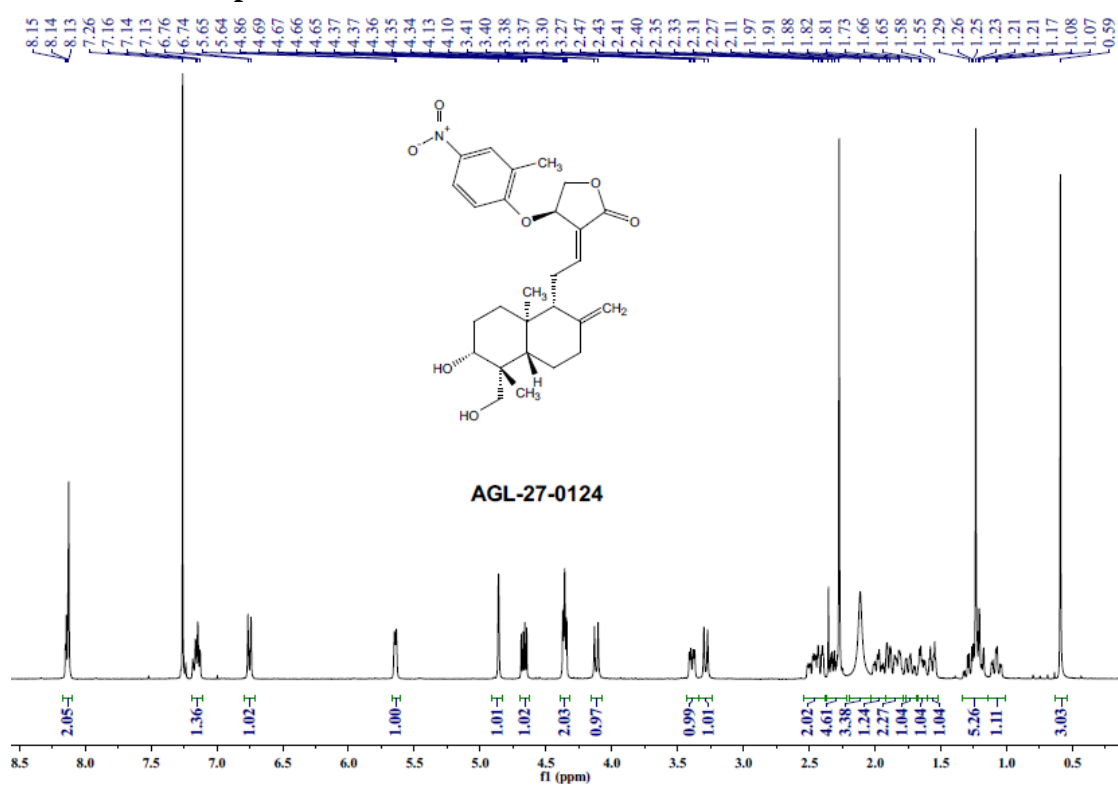
¹H NMR of Compound 12g:



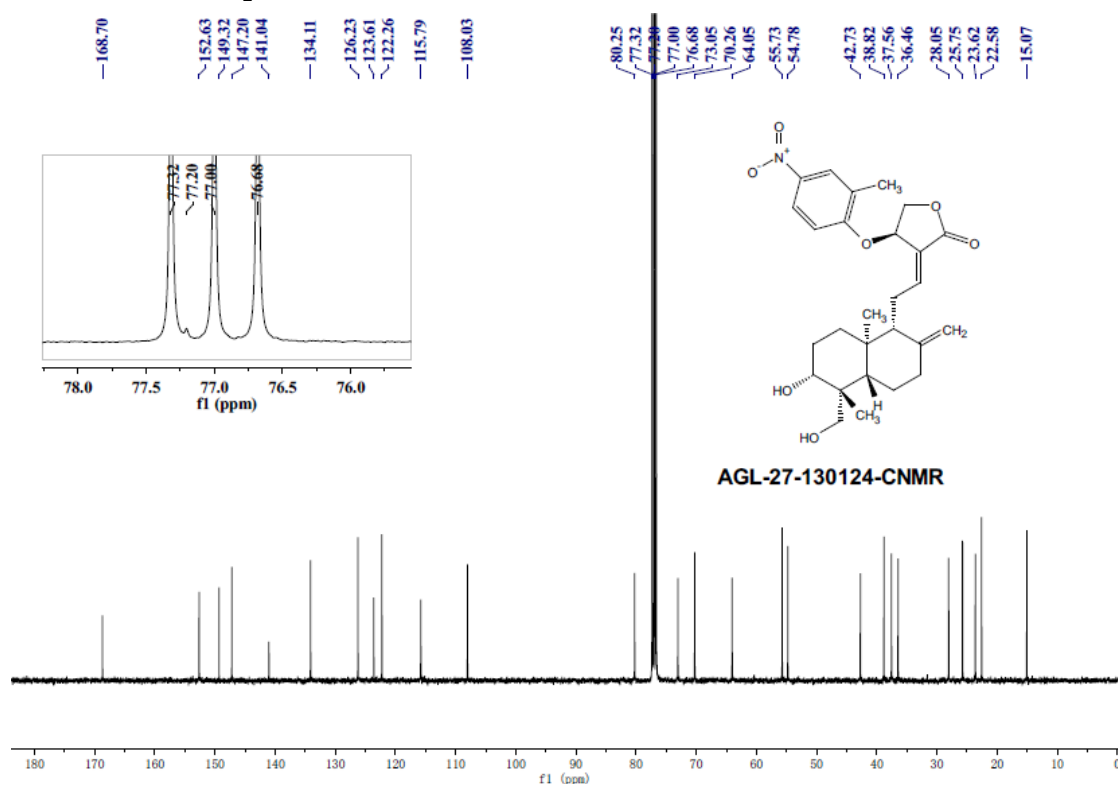
¹³C NMR of Compound 12g:



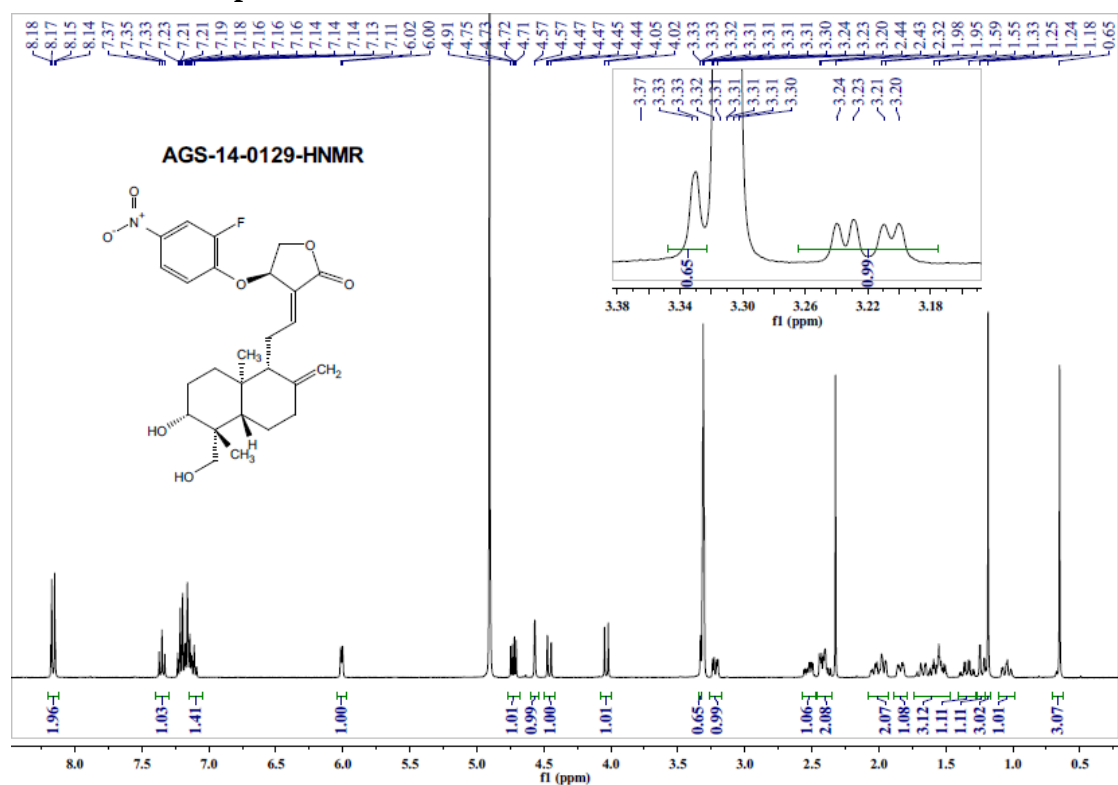
¹H NMR of Compound 12h:



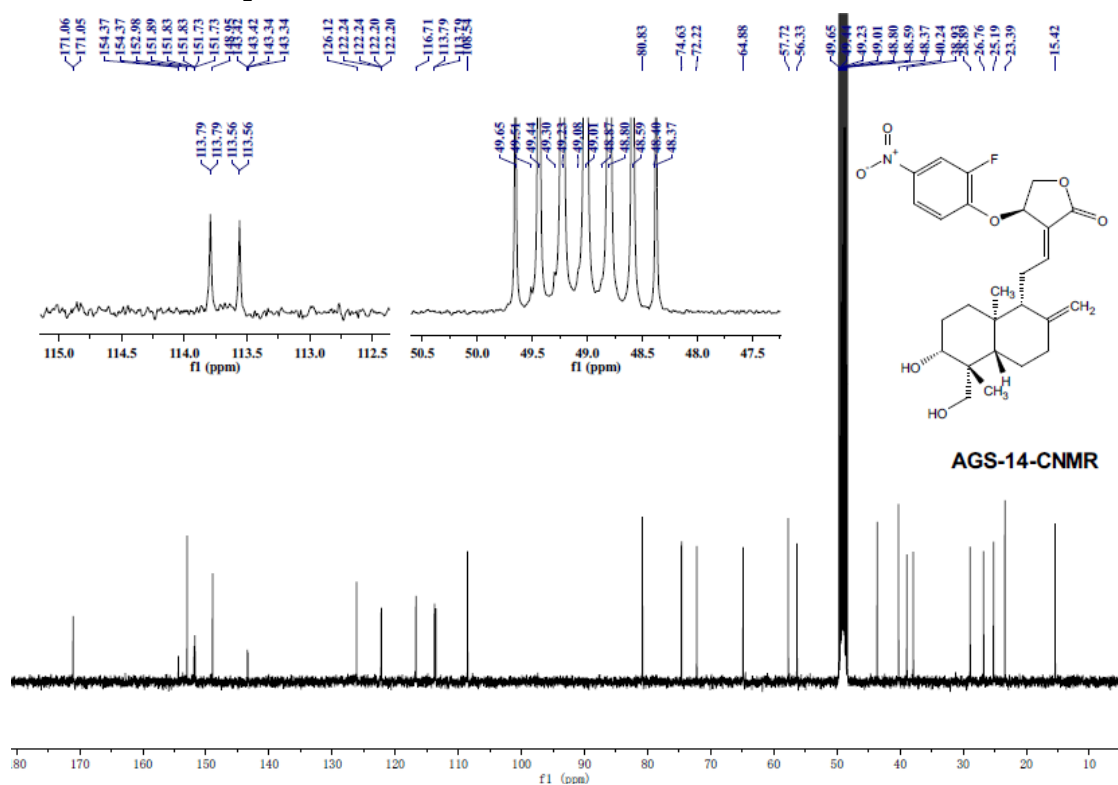
¹³C NMR of Compound 12h:



¹H NMR of Compound 12i:

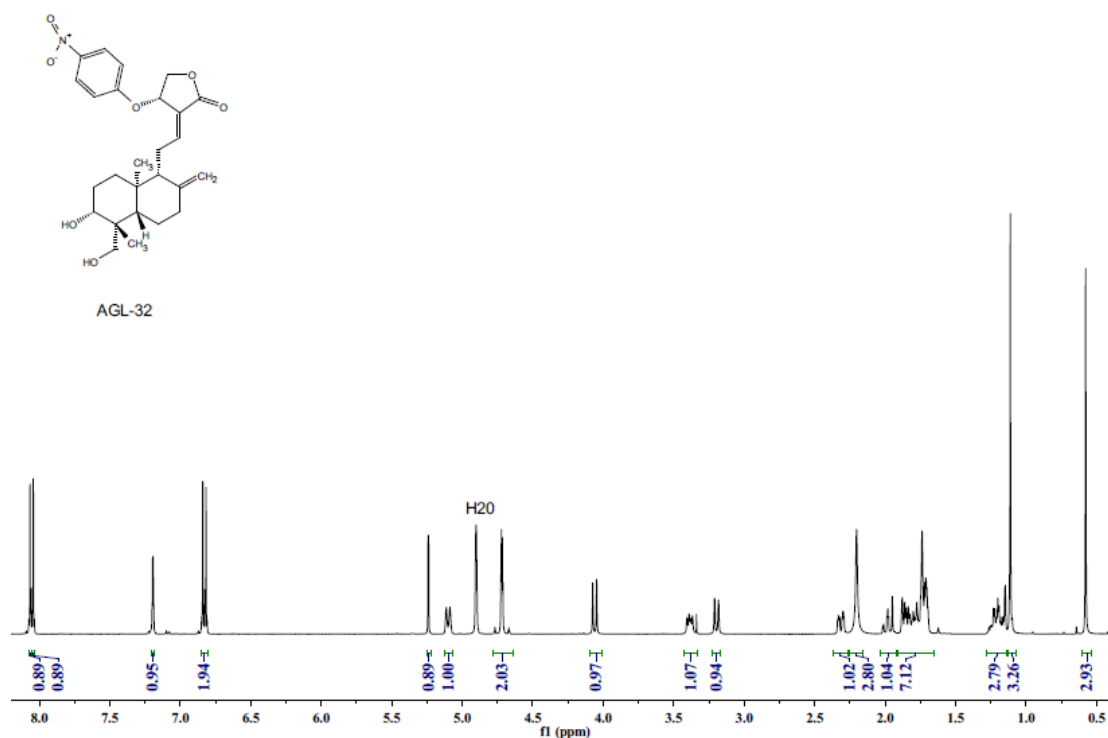


¹³C NMR of Compound 12i:



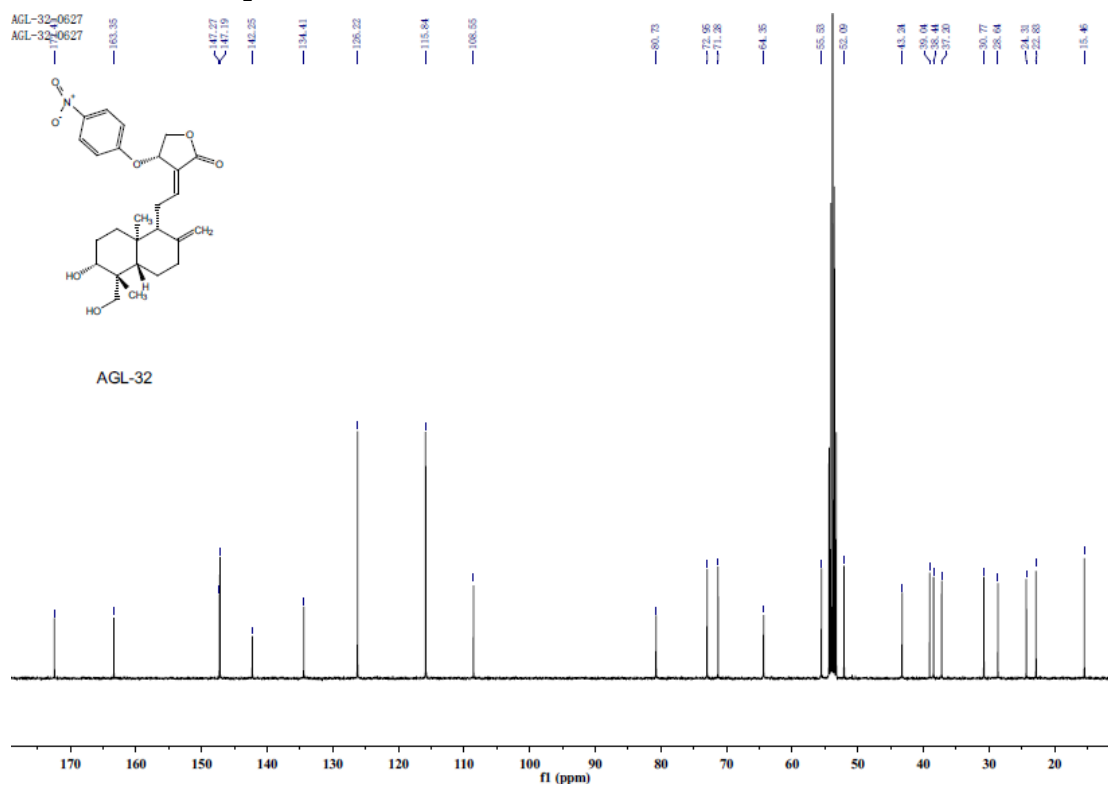
¹H NMR of Compound 13b:

AGL-32-0627
AGL-32-0627



¹³C NMR of Compound 13b:

AGL-32-0627
AGL-32-0627



Chemical structure of compound 1: CC1(C)C(C(C1)O)C(C(C2=CC(=C(C=C2)OC(=O)C)OC3=CC=CC=C3N(C)C)O)O

¹H NMR spectrum (CDCl₃):

- Chemical shift range:** 0.5 – 8.0 ppm
- Integration values:** 1.03, 0.98, 1.02, 0.99, 1.00, 1.20, 1.01, 1.01, 1.02, 1.02, 3.11, 1.41, 3.07, 2.07, 1.02, 2.11, 1.09, 1.10, 5.24, 3.05
- Peak assignments (ppm):** 7.93, 7.92, 7.91, 7.90, 7.88, 7.88, 7.14, 7.11, 7.05, 7.05, 7.04, 7.03, 7.03, 7.02, 7.02, 5.84, 5.82, 4.87, 4.87, 4.83 (HDO), 4.72, 4.70, 4.69, 4.67, 4.64, 4.63, 4.44, 4.43, 4.41, 4.41, 4.07, 4.04, 3.94, 3.36, 3.35, 3.33 (MeOD), 3.33 (MeOD), 3.32 (MeOD), 3.31 (MeOD), 3.30 (MeOD), 3.30 (MeOD), 2.49, 2.47, 2.46, 2.44, 2.43, 2.43, 2.42, 2.40, 2.39, 2.39, 2.00, 1.97, 1.94, 1.71, 1.70, 1.69, 1.68, 1.67, 1.62, 1.39, 1.38, 1.33, 1.33, 1.26, 1.23, 1.23, 1.21, 1.20, 1.19, 0.62

AGN-3-CNMR

Chemical shift labels (ppm):

- 171.45
- 153.12
- 152.55
- 151.95
- 148.73
- 126.18
- 118.28
- 116.58
- 109.48
- 108.45
- 80.89
- 74.76
- 72.59
- 64.92
- 57.18
- 56.87
- 56.30
- 49.65
- 49.44
- 49.22
- 49.01
- 48.80
- 48.59
- 48.37
- 26.37
- 25.18
- 23.36
- 15.44

Peak labels (ppm):

- 153.12
- 152.55
- 151.95
- 57.18
- 56.87
- 56.30
- 49.65
- 49.44
- 49.22
- 49.01
- 48.80
- 48.59
- 48.37