

Supplementary Material

Design, semisynthesis and estrogenic activity of lignan derivatives from natural dibenzylbutyrolactones

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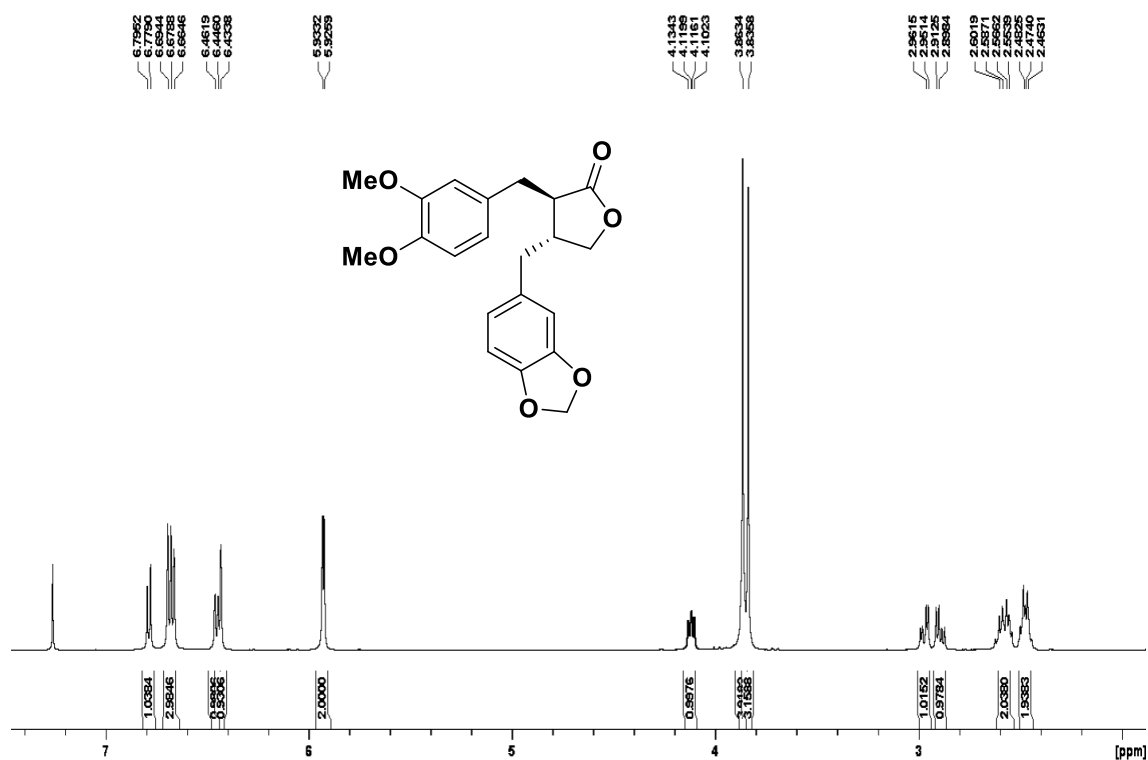
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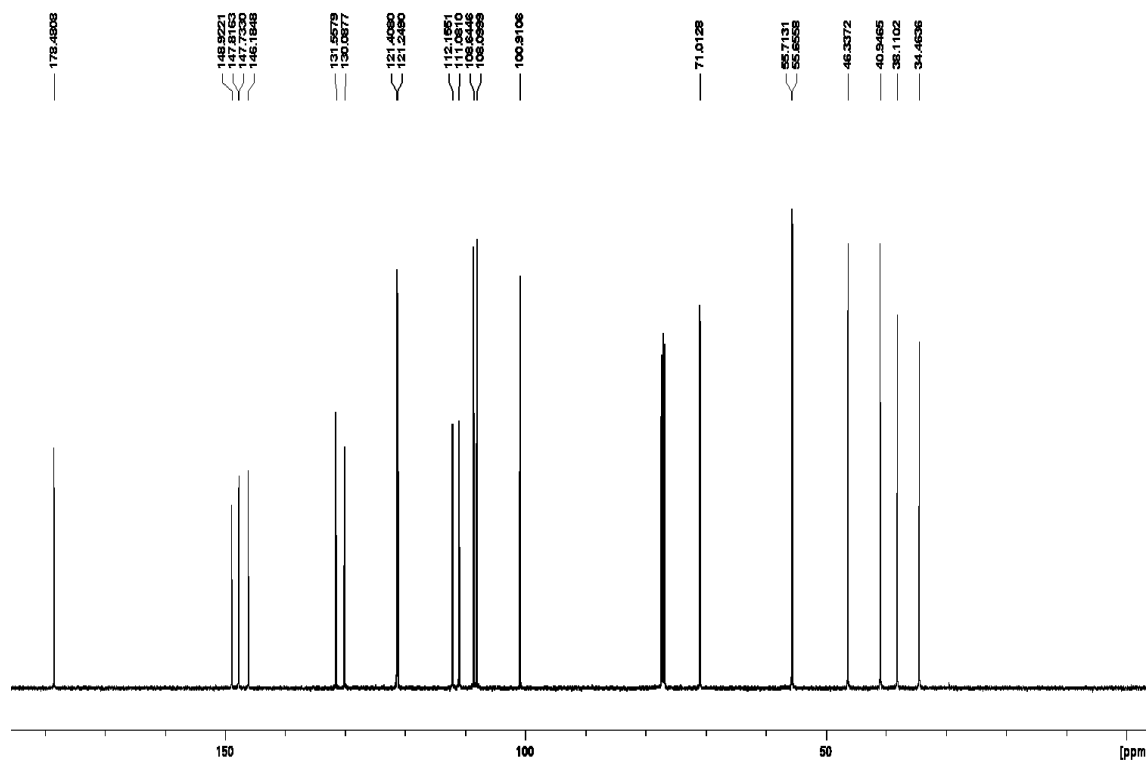
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¹H-NMR and ¹³C-NMR spectra of compounds **1-16**.

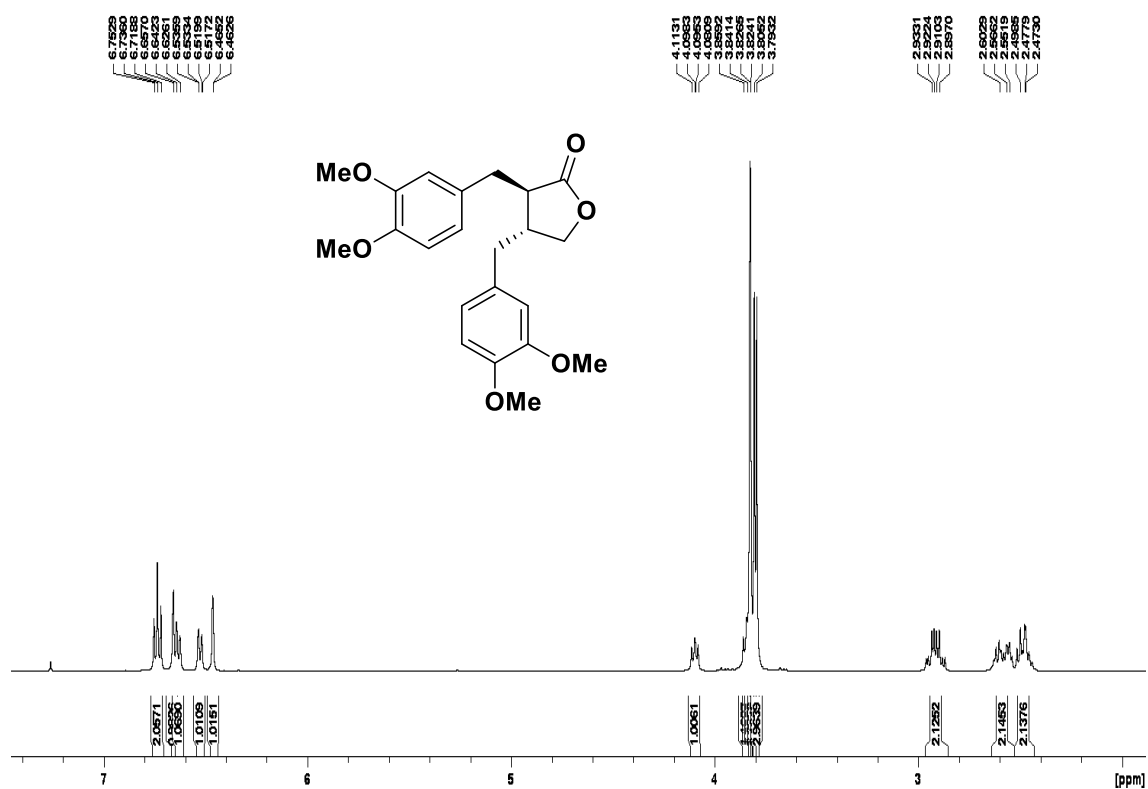
^1H -NMR (CDCl_3 , 500 MHz) of (–)-bursehernin (**1**).



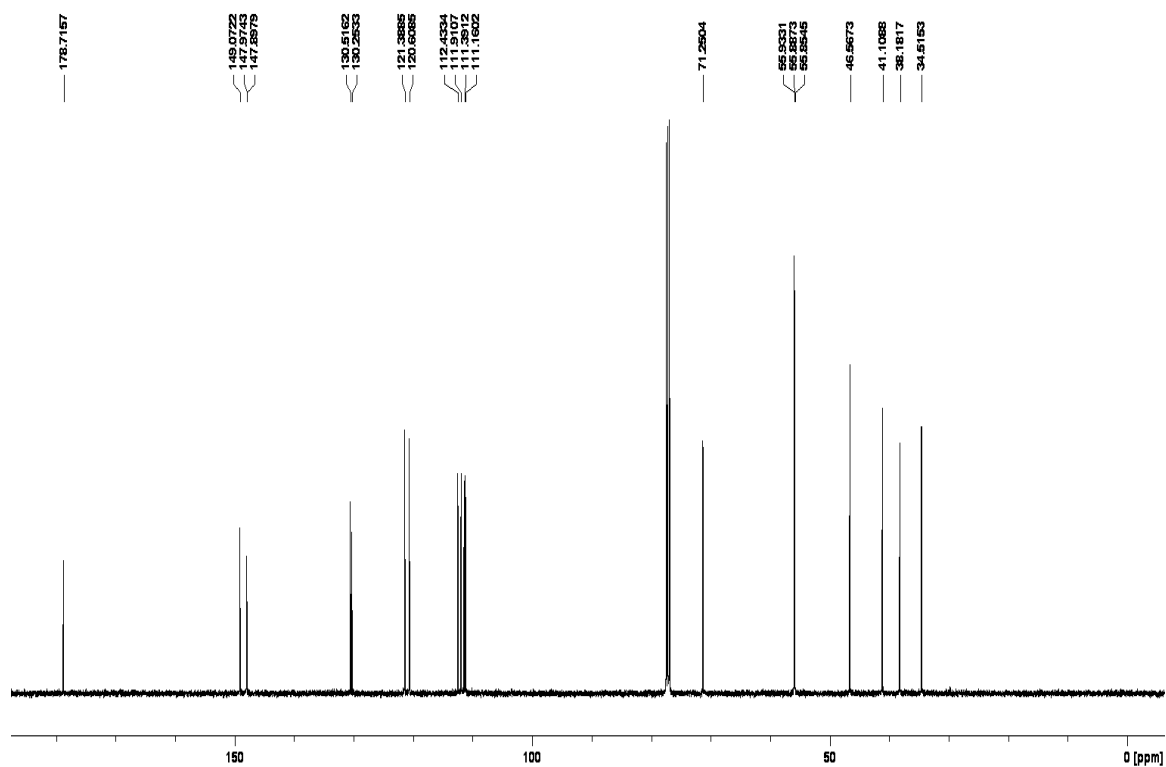
^{13}C -NMR (CDCl_3 , 500 MHz) of (–)-bursehernin (**1**).



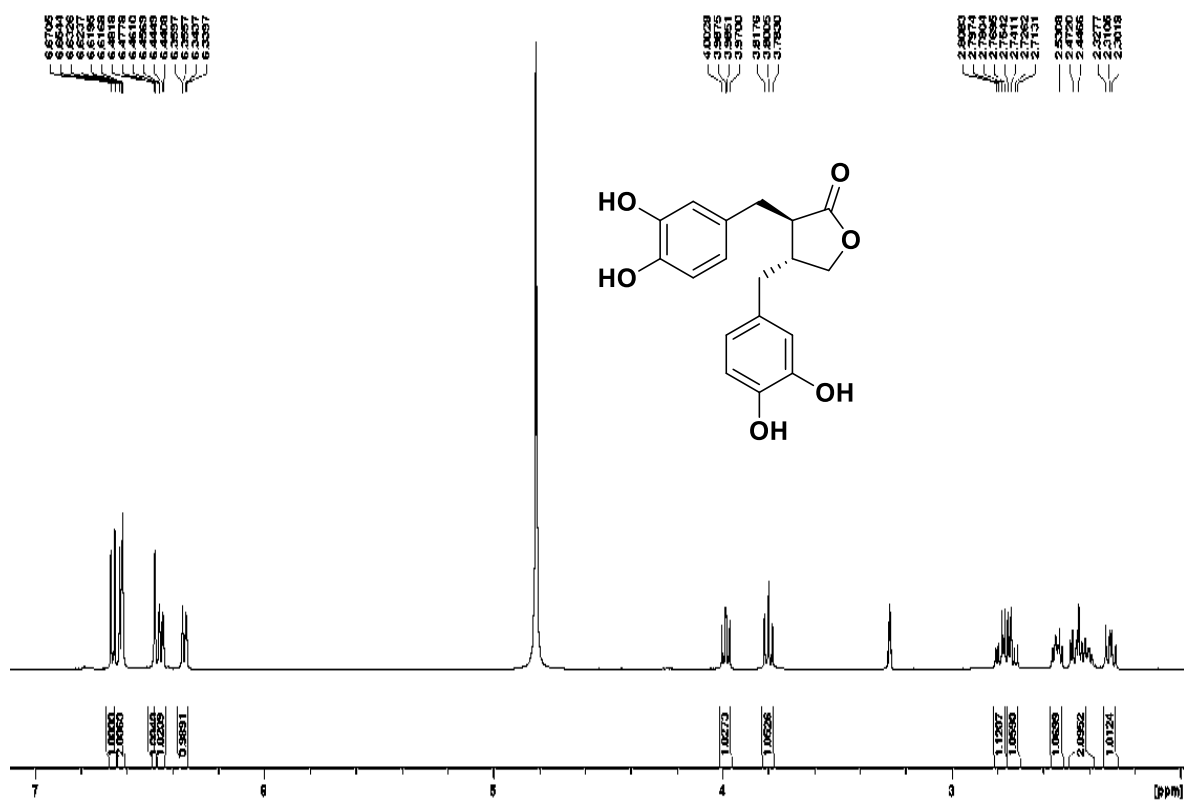
^1H -NMR (CDCl_3 , 500 MHz) of (–)-matairesinol dimethyl ether (2).



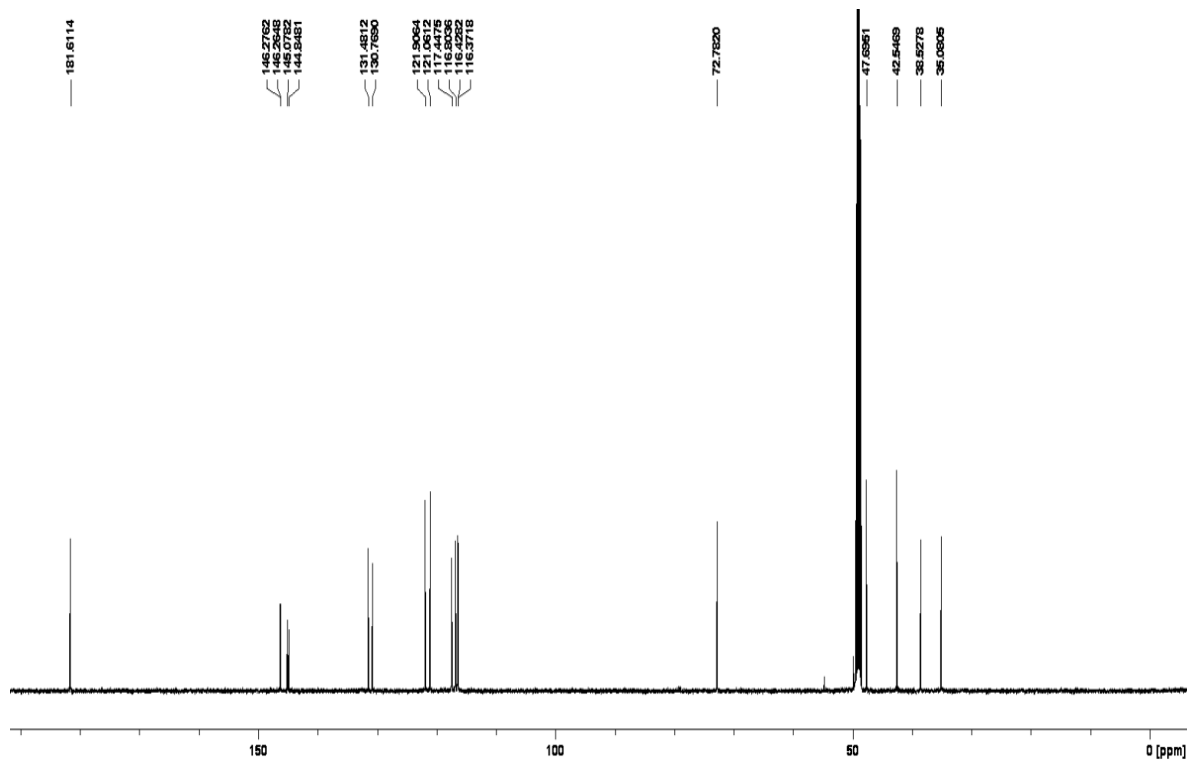
^{13}C -NMR (CDCl_3 , 500 MHz) of (–)-matairesinol dimethyl ether (2).



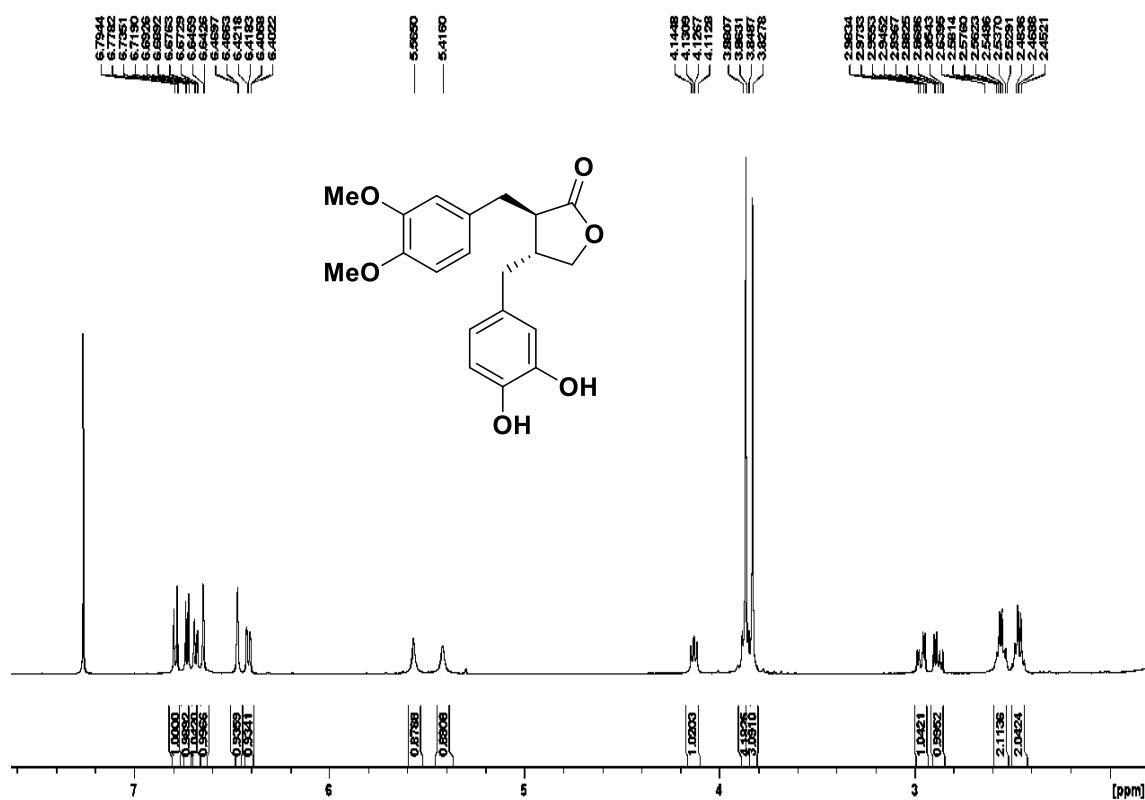
^1H -NMR (MeOD- d_4 , 500 MHz) of compound **3**.



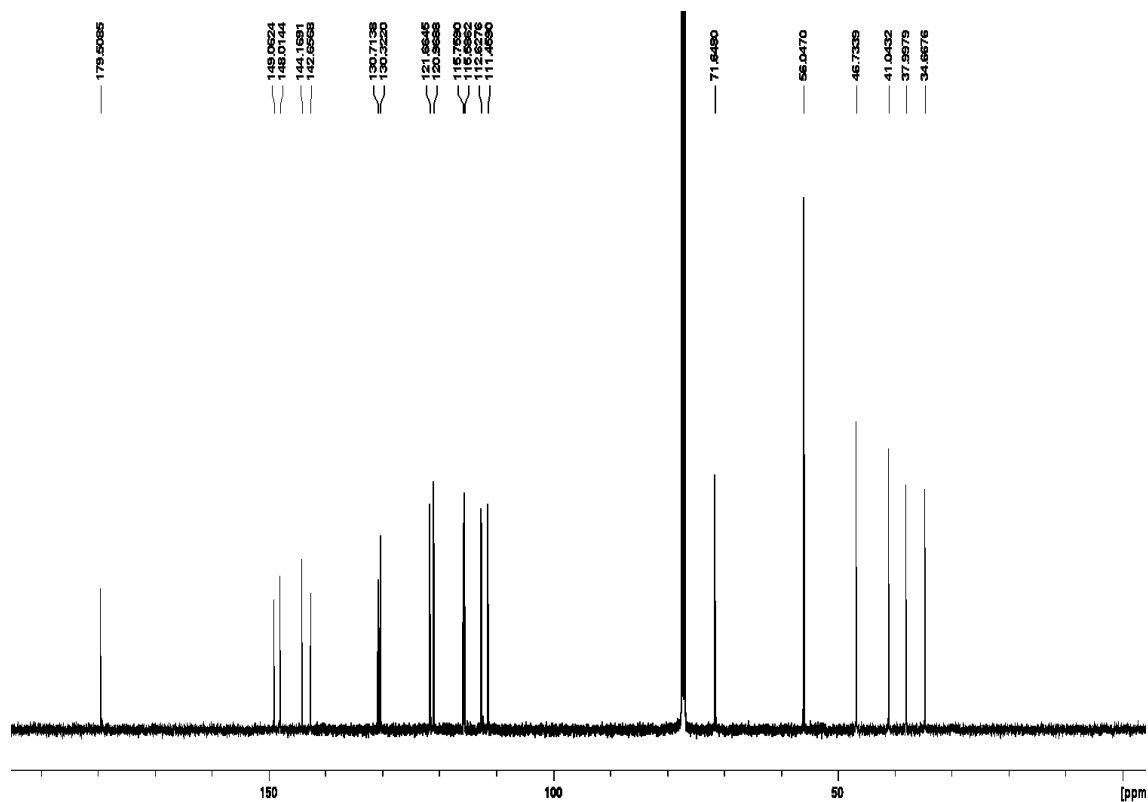
^{13}C -NMR (MeOD- d_4 , 500 MHz) of compound **3**.



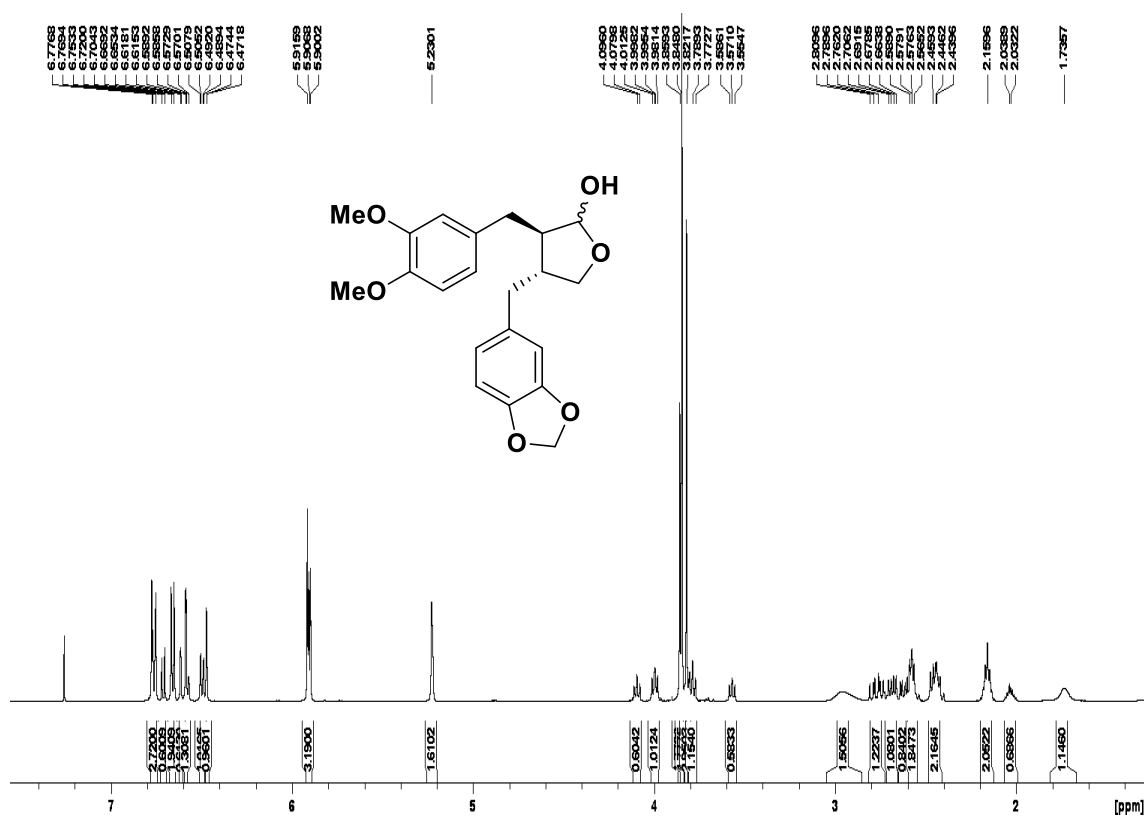
^1H -NMR (CDCl_3 , 500 MHz) of compound 4.



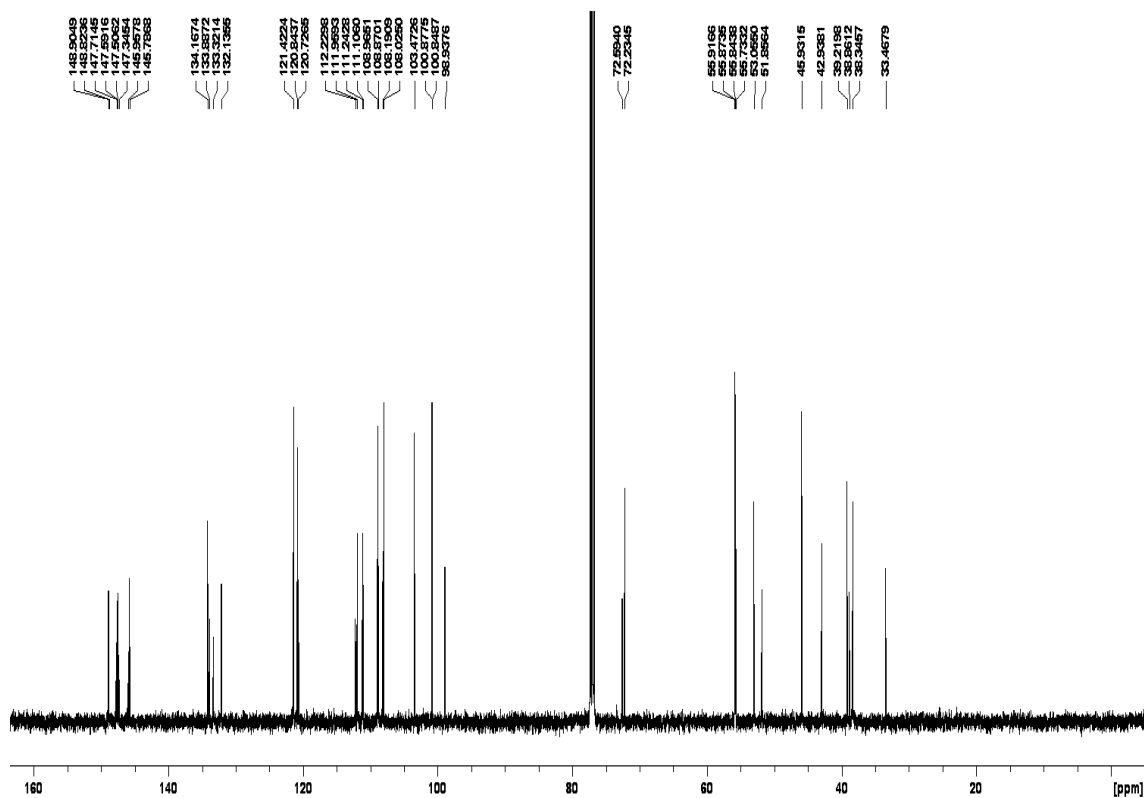
^{13}C -NMR (CDCl_3 , 500 MHz) of compound 4.



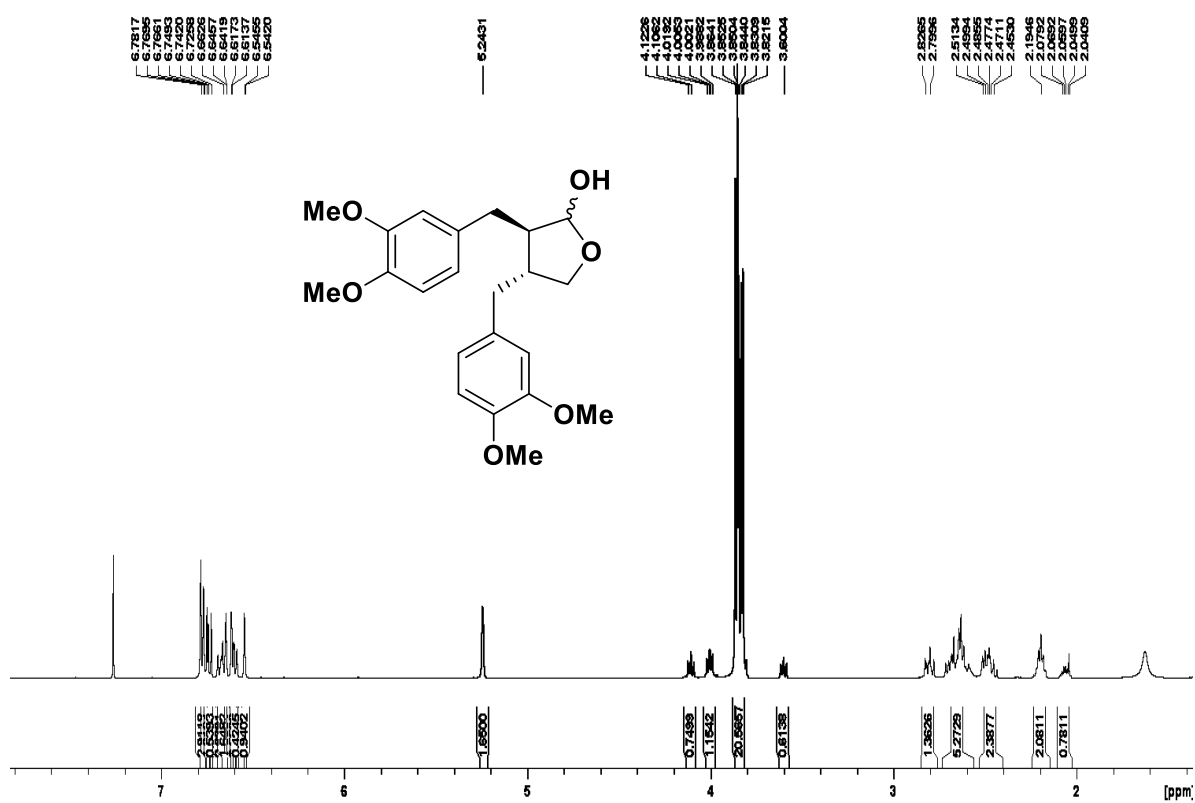
$^1\text{H-NMR}$ (CDCl_3 , 500 MHz) of compound **5**.



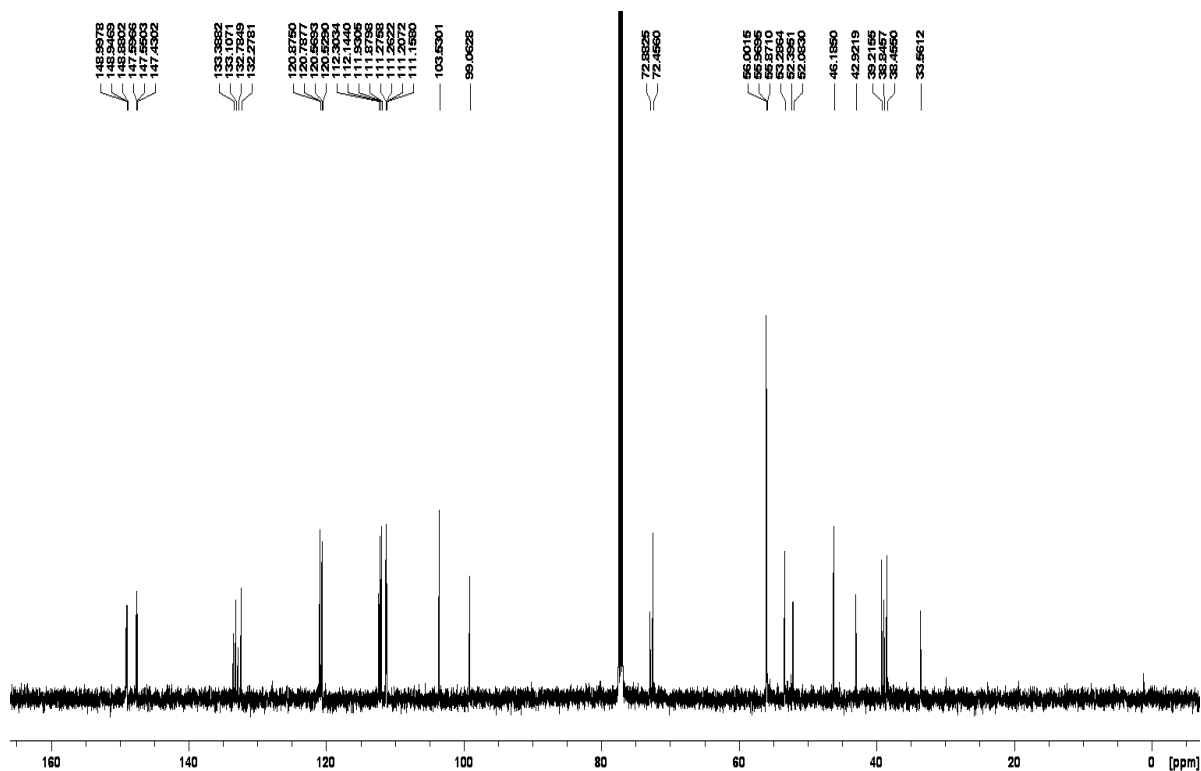
$^{13}\text{C-NMR}$ (CDCl_3 , 500 MHz) of compound **5**.



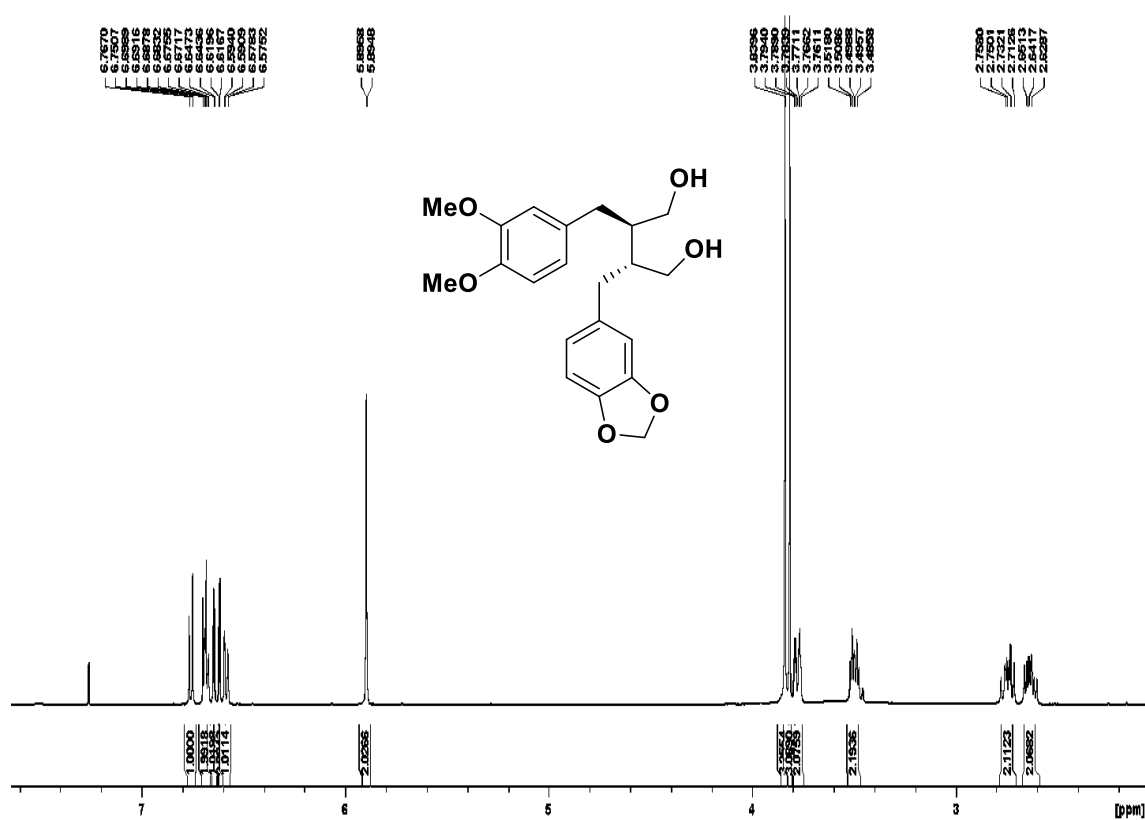
^1H -NMR (CDCl_3 , 500 MHz) of compound 6.



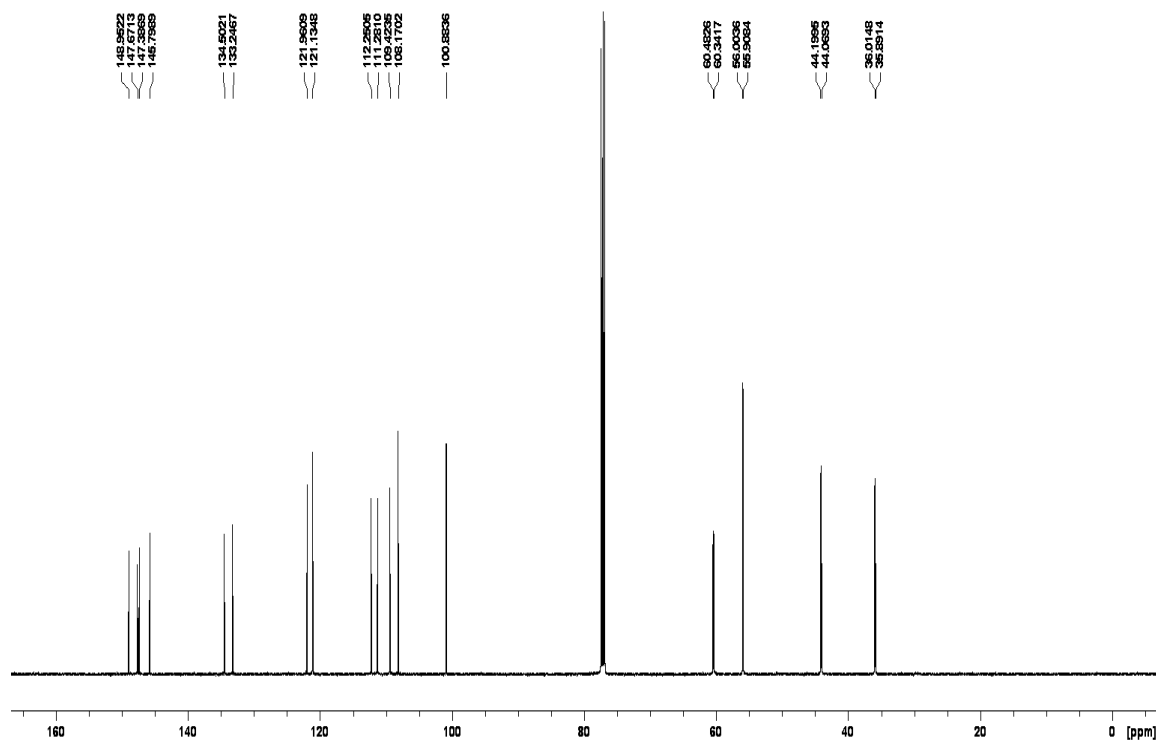
^{13}C -NMR (CDCl_3 , 500 MHz) of compound 6.



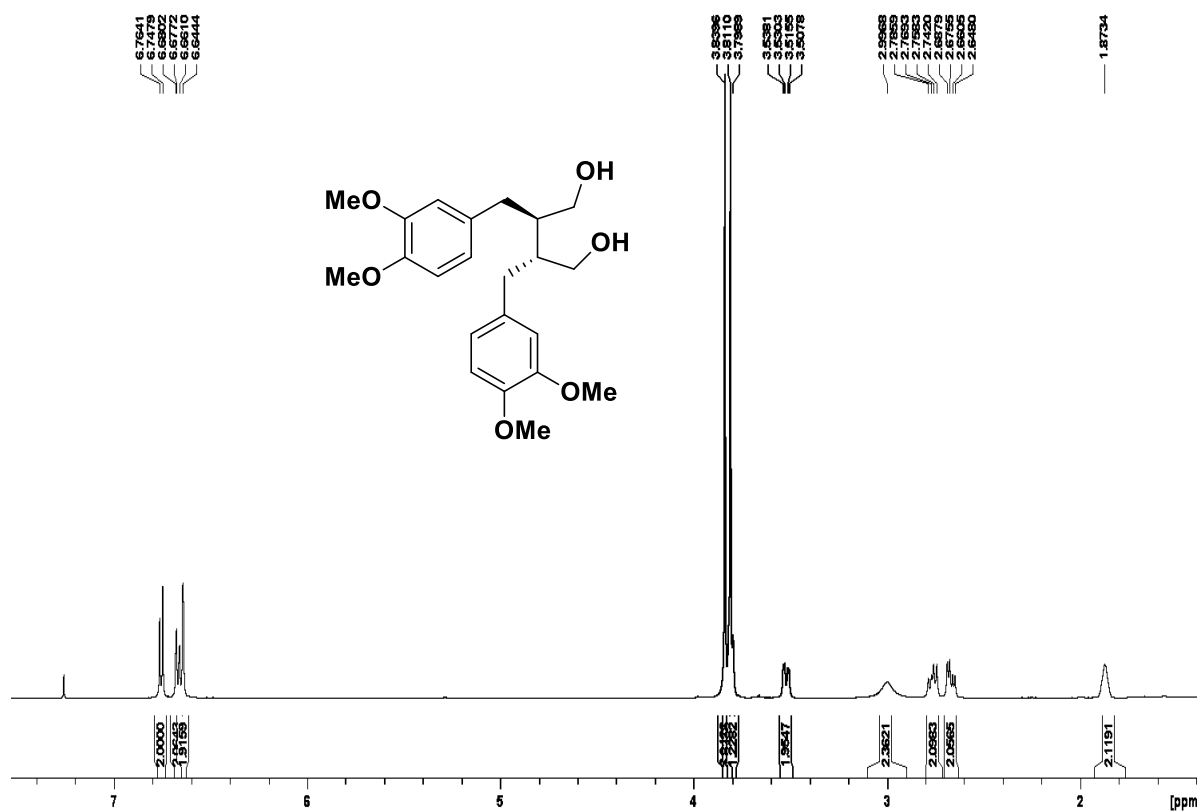
^1H -NMR (CDCl_3 , 500 MHz) of compound 7.



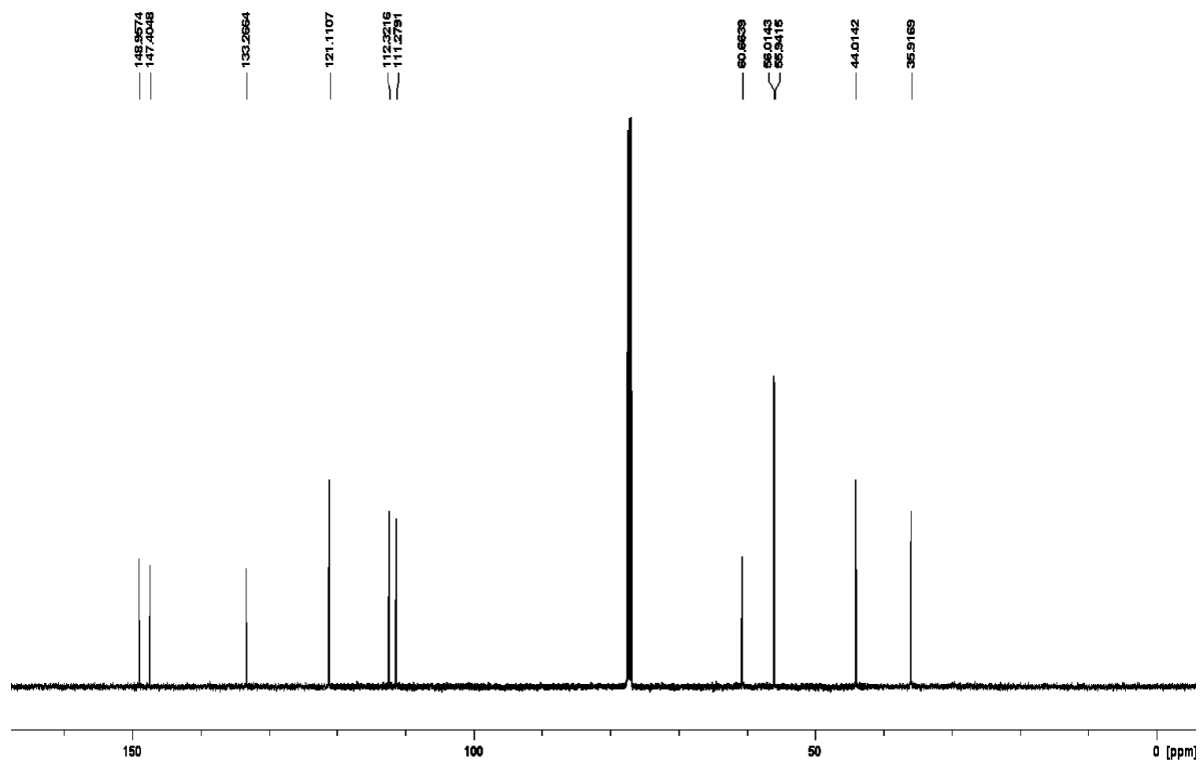
^{13}C -NMR (CDCl_3 , 500 MHz) of compound 7.



^1H -NMR (CDCl_3 , 500 MHz) of compound **8**.



^{13}C -NMR (CDCl_3 , 500 MHz) of compound **8**.



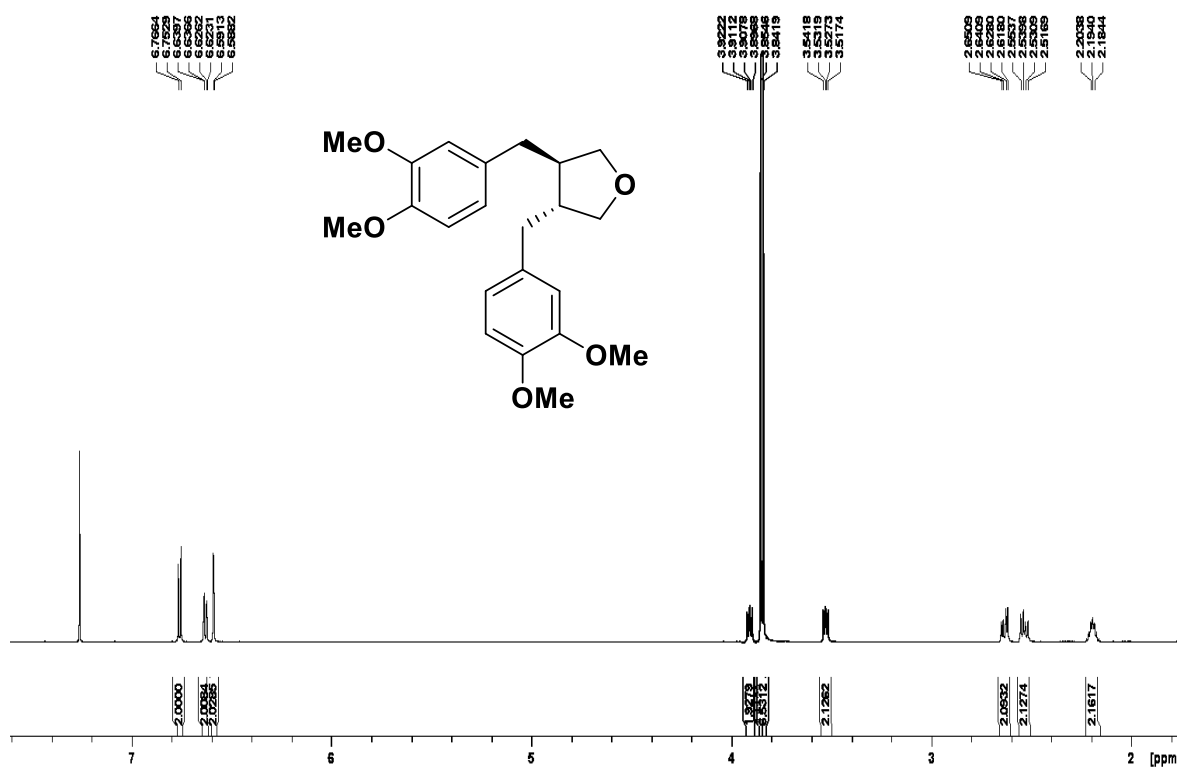
Chemical structure of compound 10 is shown above the spectrum. The structure is a 3,4-dimethoxyphenyl group attached to a 1,3-dioxolane ring, which is further attached to a 1,3-benzodioxole ring.

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 0 to 8 ppm. The chemical shifts and integrations are listed below the spectrum:

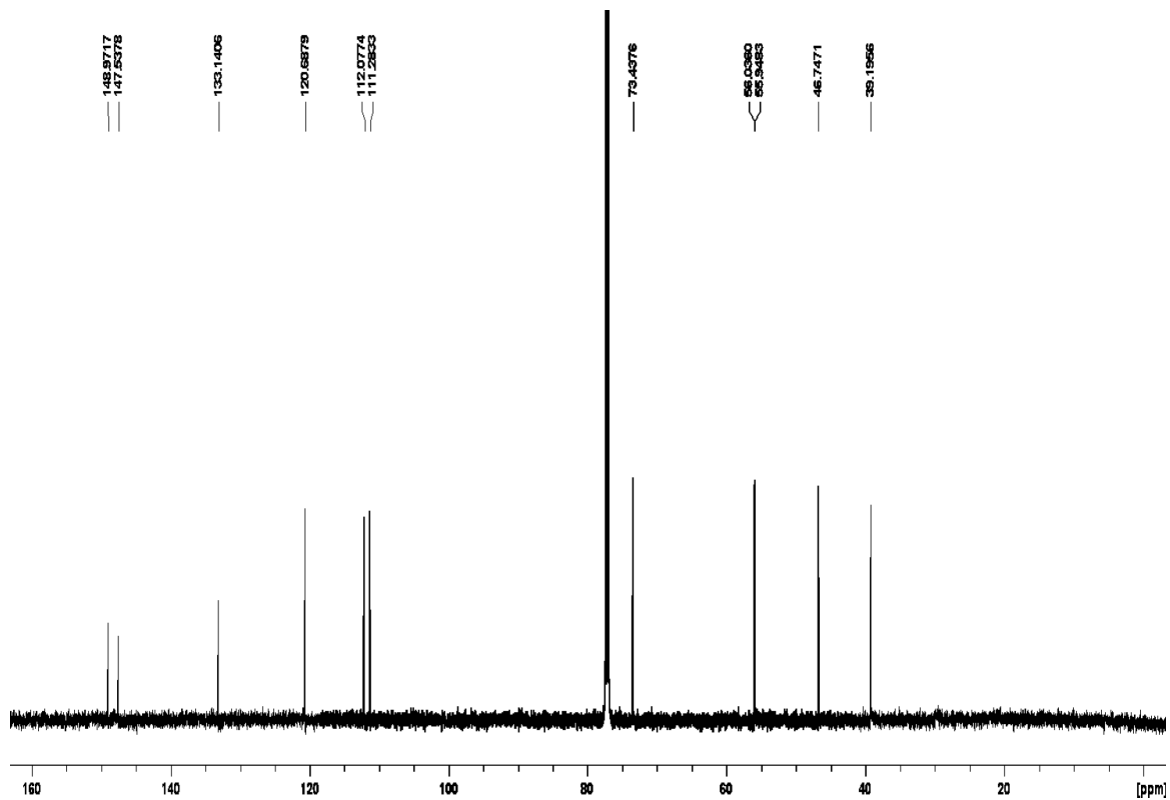
Chemical Shift (ppm)	Integration
7.7733	1.0007
7.7574	1.0028
7.7532	1.0028
7.6460	1.0028
7.5706	1.0027
7.5407	1.0027
7.5236	1.0027
5.9217	2.0000
3.9034	2.1828
3.8409	2.3116
3.8194	1.9754
3.8062	1.9754
2.5953	2.0059
2.5852	2.0023
2.5765	2.0023
2.5642	2.0023
2.5402	2.0023
2.5251	2.0023
2.5163	2.0023
2.4963	2.0023
2.1674	2.0341

149.0033
147.7723
146.9625
146.5655
134.2900
133.0924
121.6170
120.7200
111.9695
111.3157
108.1009
106.1803
100.5863
73.4651
73.4071
56.0357
55.9141
46.7951
46.6527
39.3111
39.2277

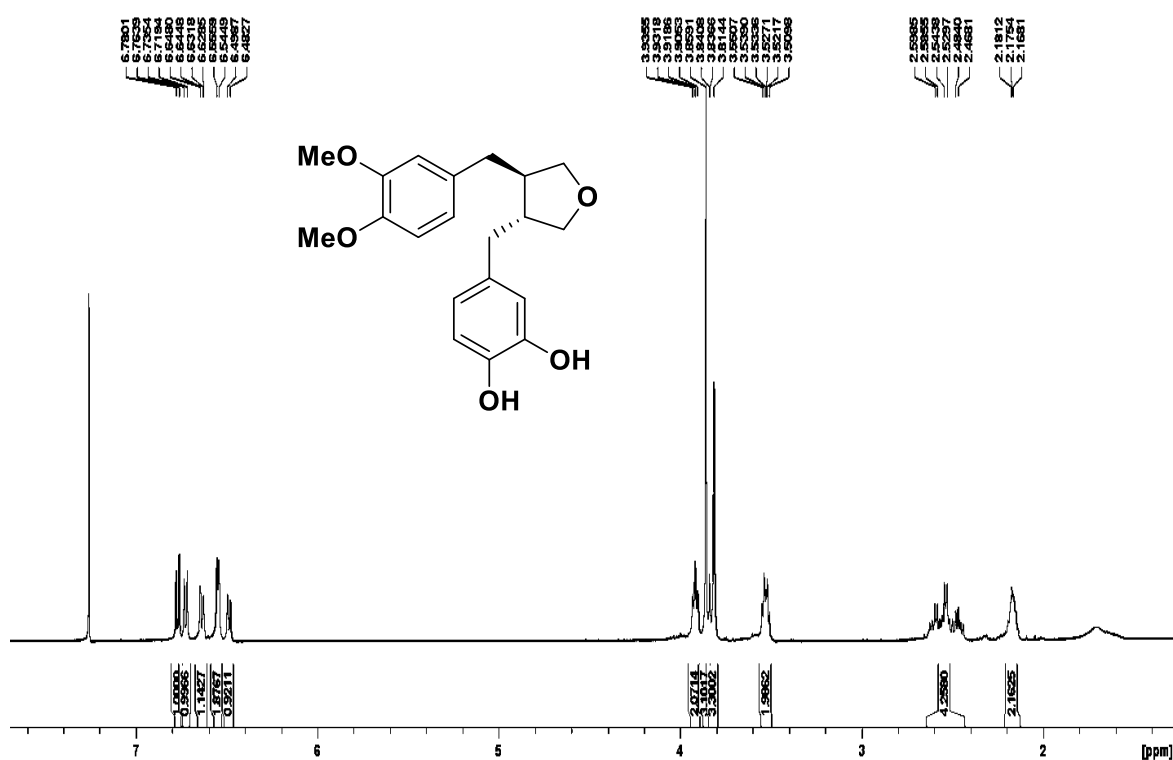
^1H -NMR (CDCl_3 , 500 MHz) of compound **10**.



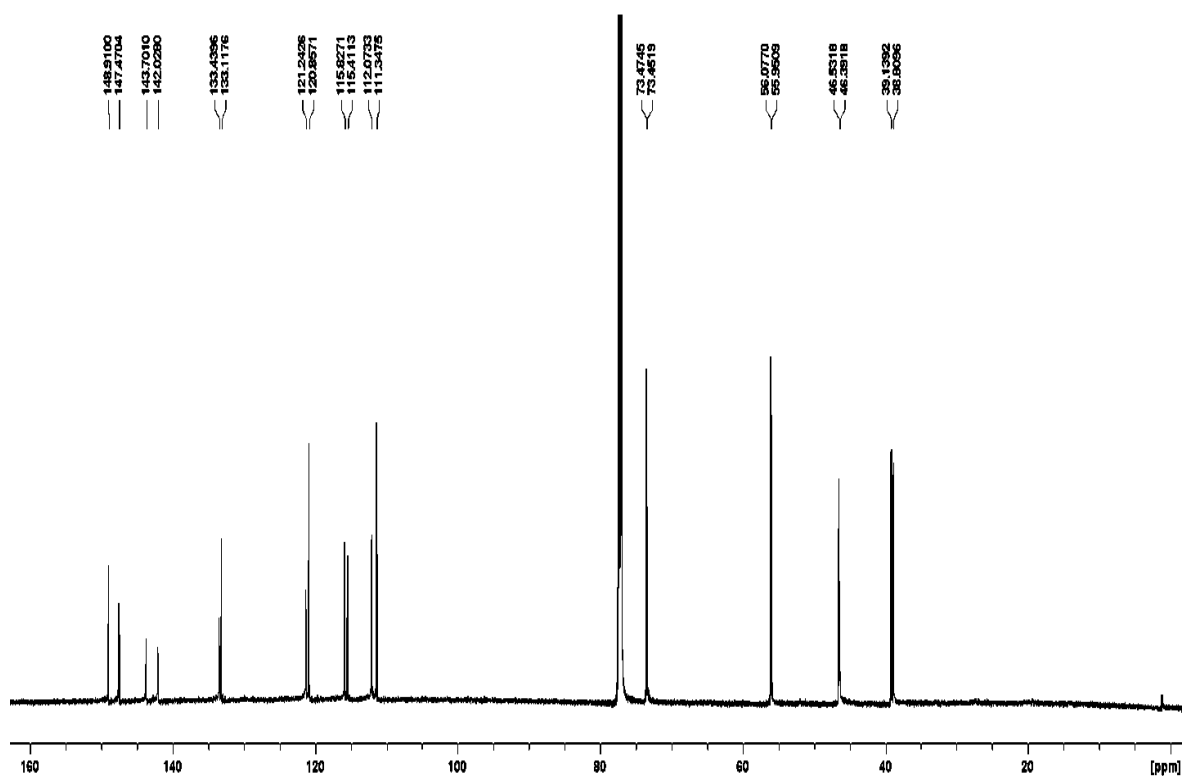
^{13}C -NMR (CDCl_3 , 500 MHz) of compound **10**.



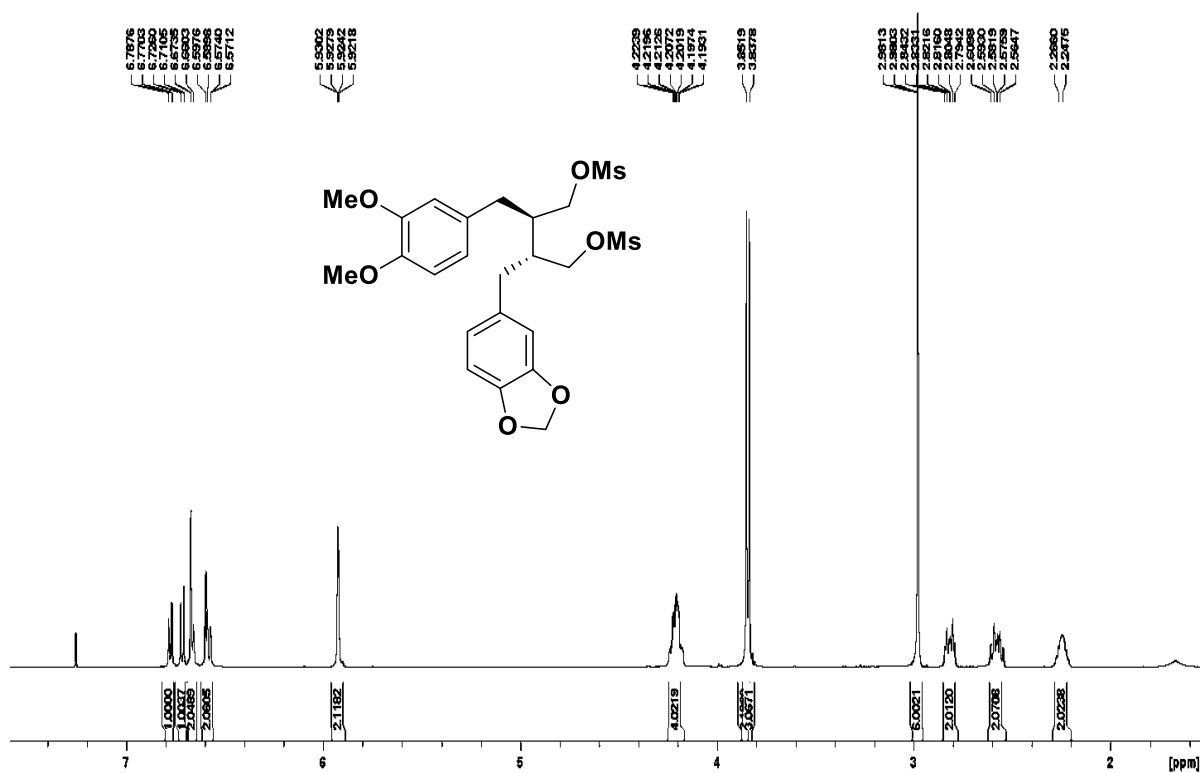
$^1\text{H-NMR}$ (CDCl_3 , 500 MHz) of compound **11**.



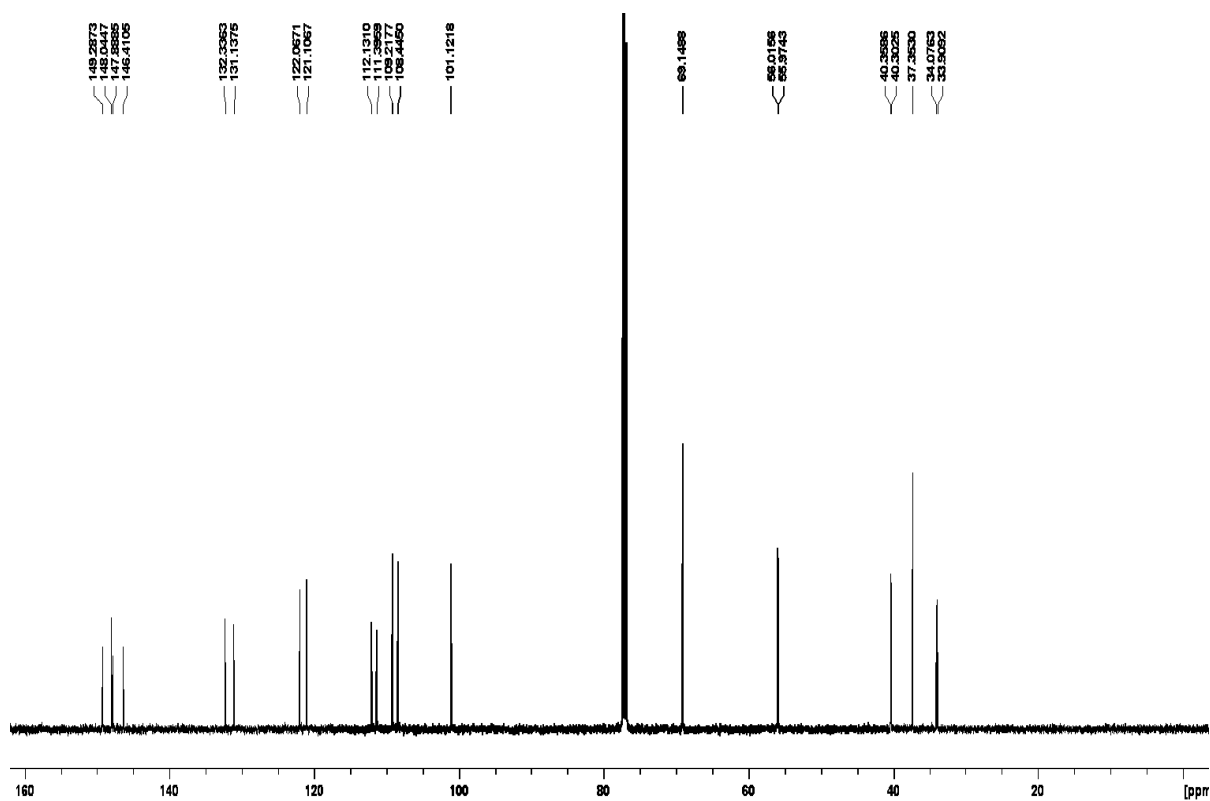
$^{13}\text{C-NMR}$ (CDCl_3 , 500 MHz) of compound **11**.



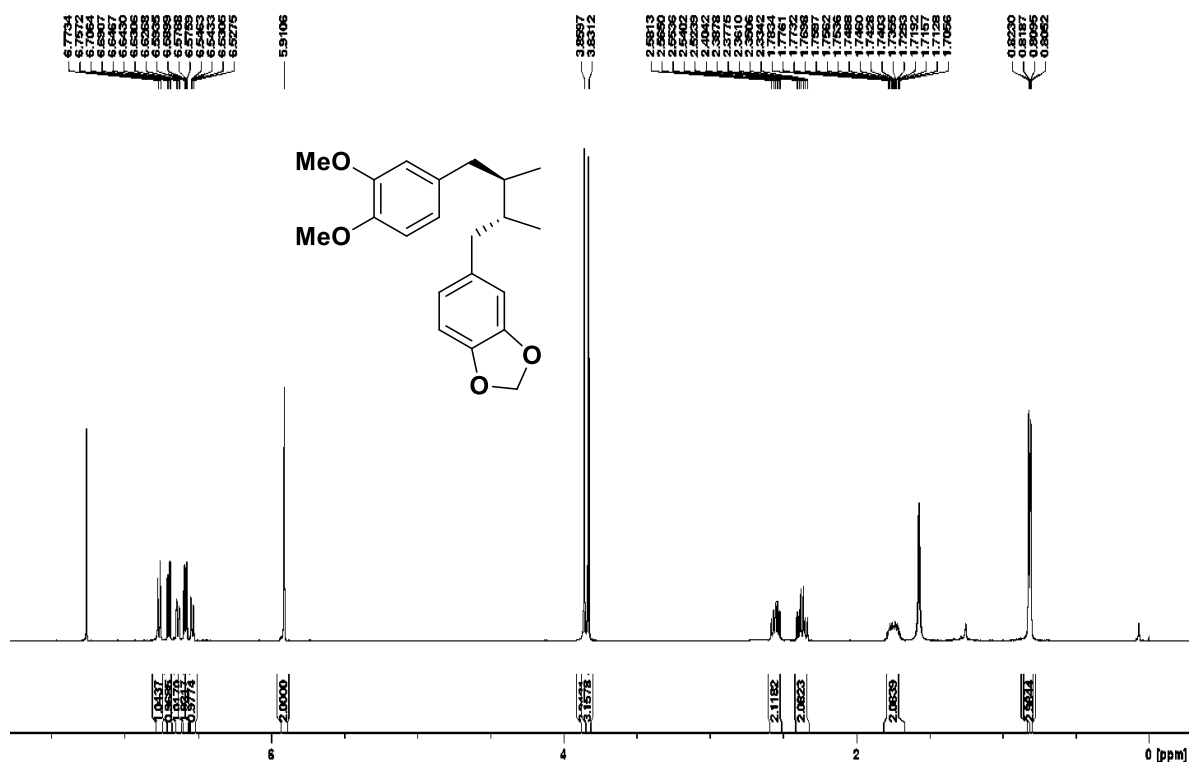
^1H -NMR (CDCl_3 , 500 MHz) of compound **12**.



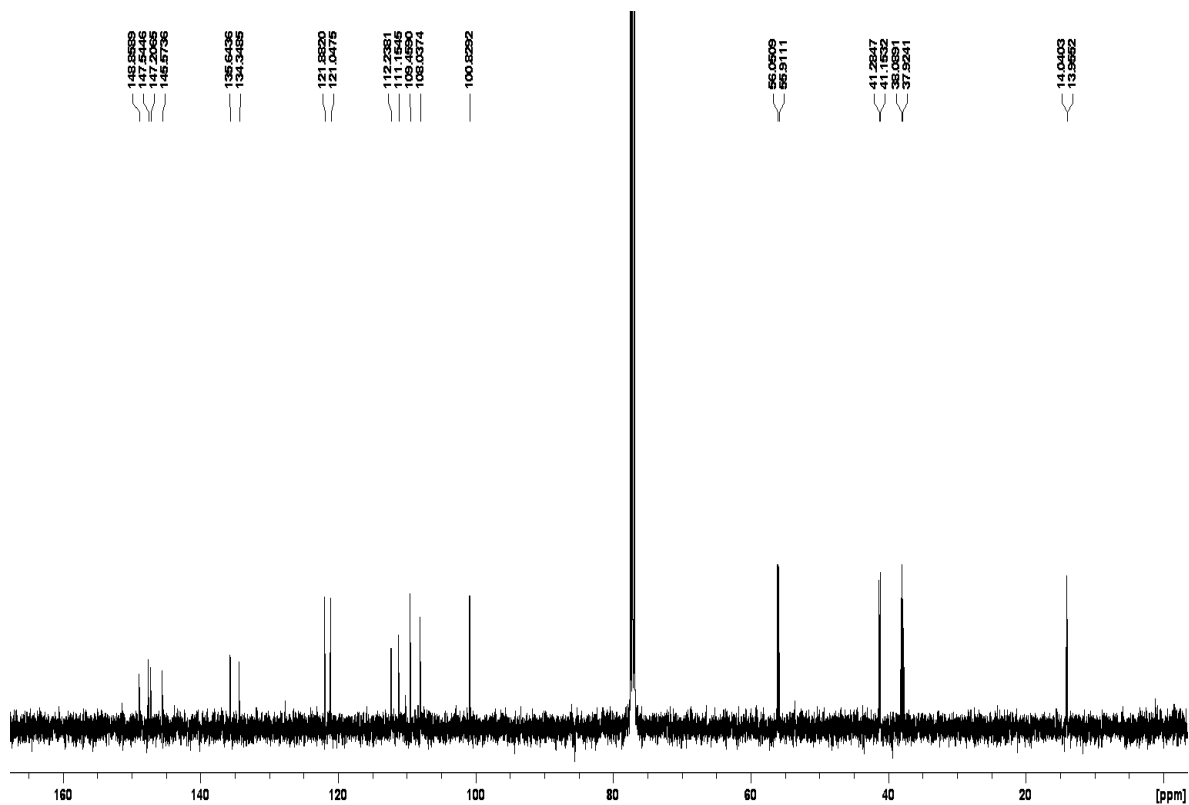
^{13}C -NMR (CDCl_3 , 500 MHz) of compound **12**.



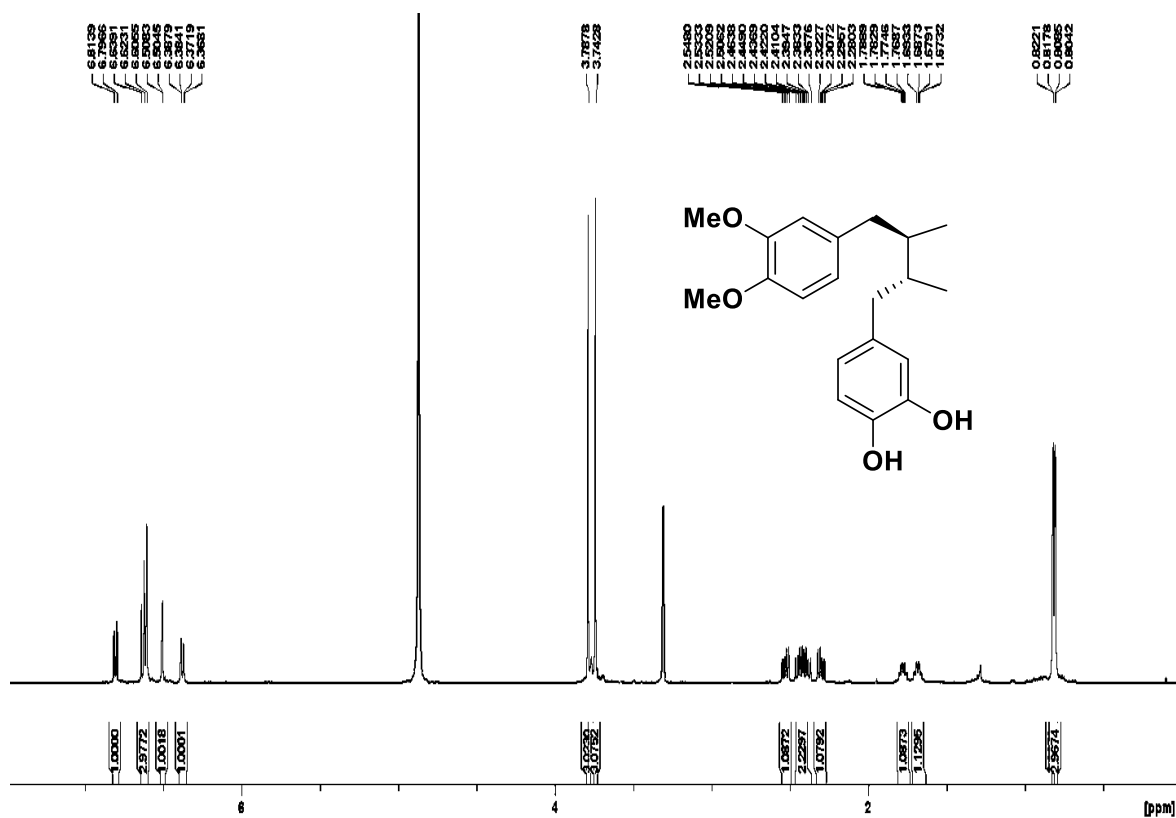
^1H -NMR (CDCl_3 , 500 MHz) of compound **13**.



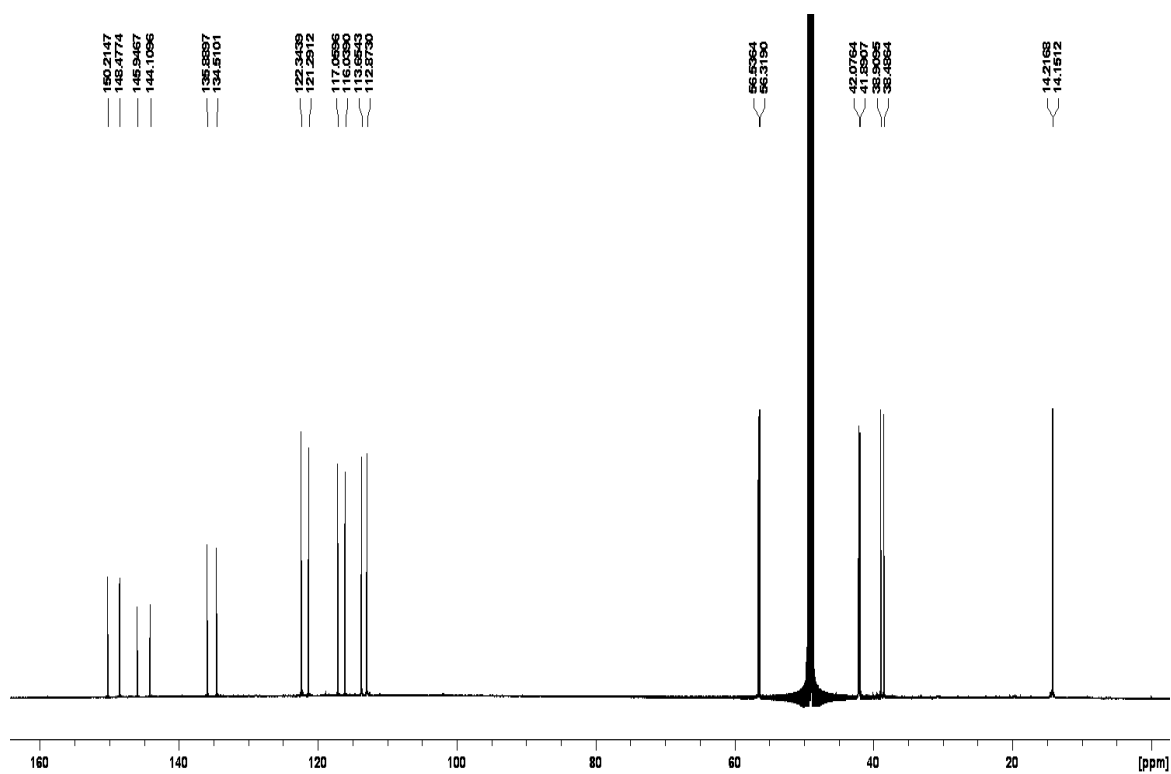
^{13}C -NMR (CDCl_3 , 500 MHz) of compound **13**.



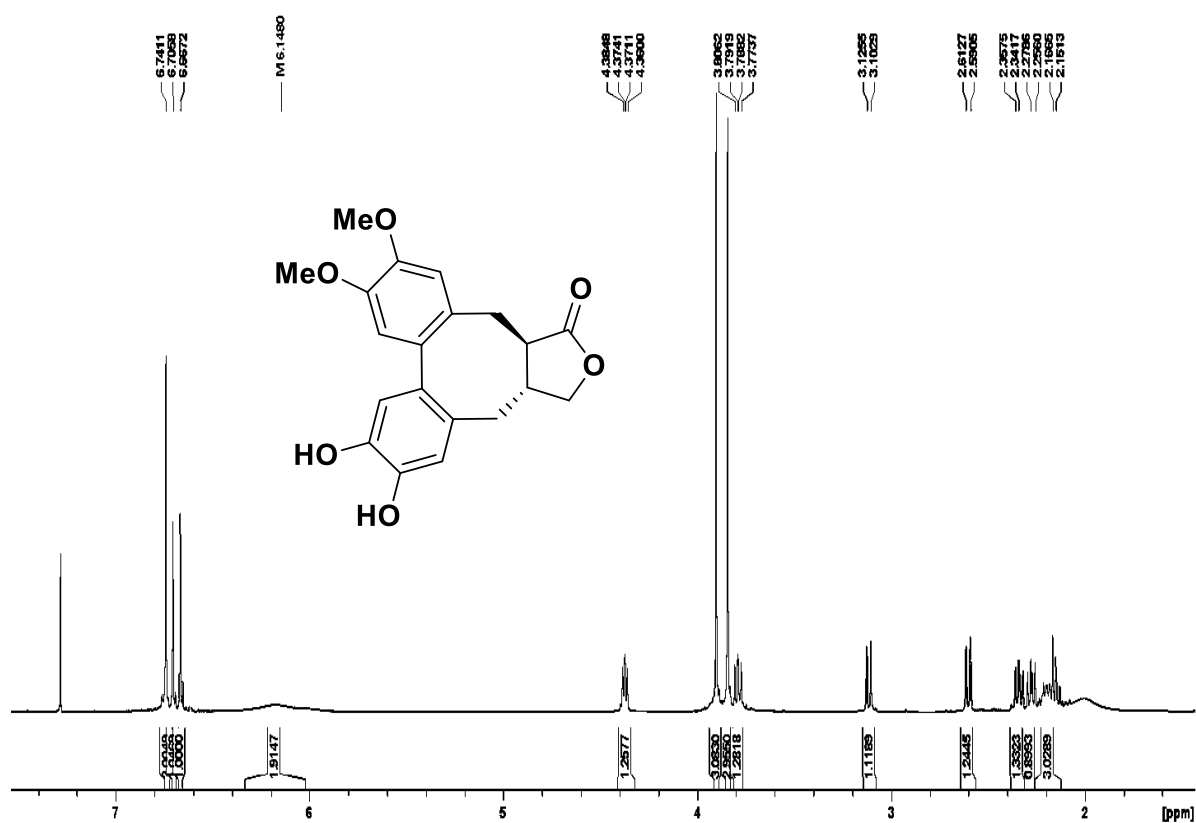
^1H -NMR (MeOD- d_4 , 500 MHz) of compound **14**.



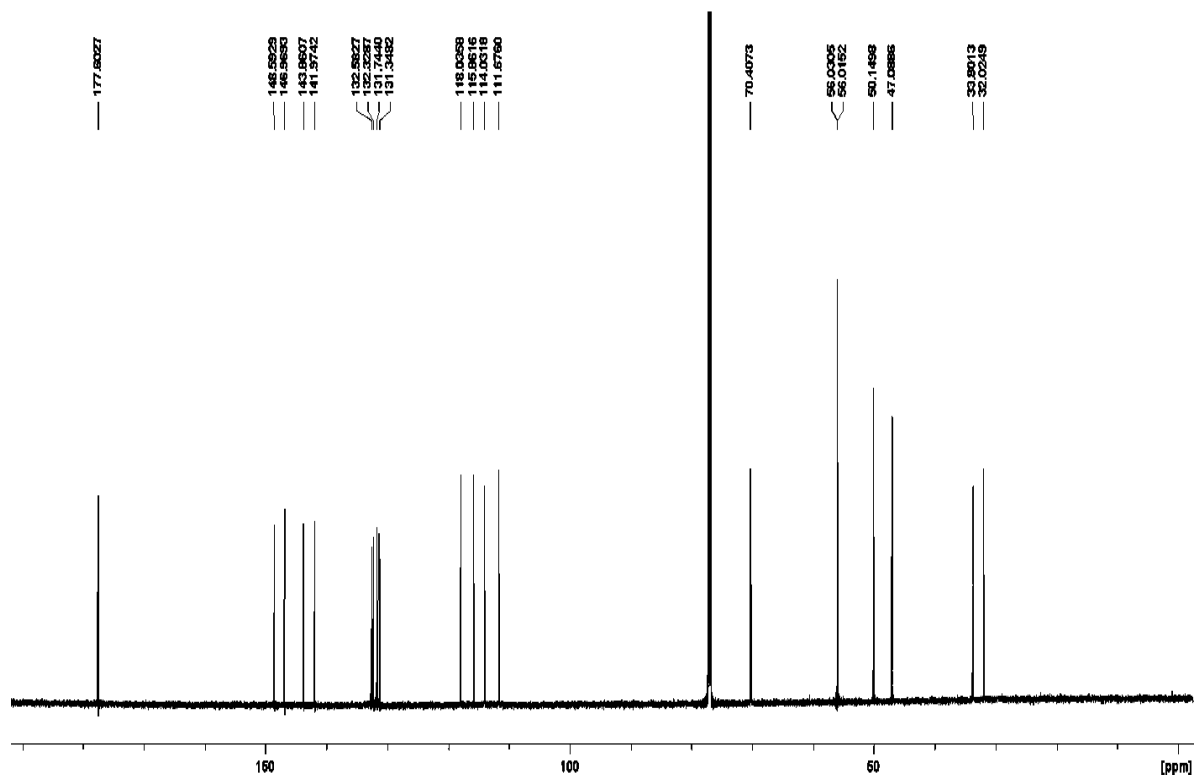
^{13}C -NMR (MeOD- d_4 , 500 MHz) of compound **14**.



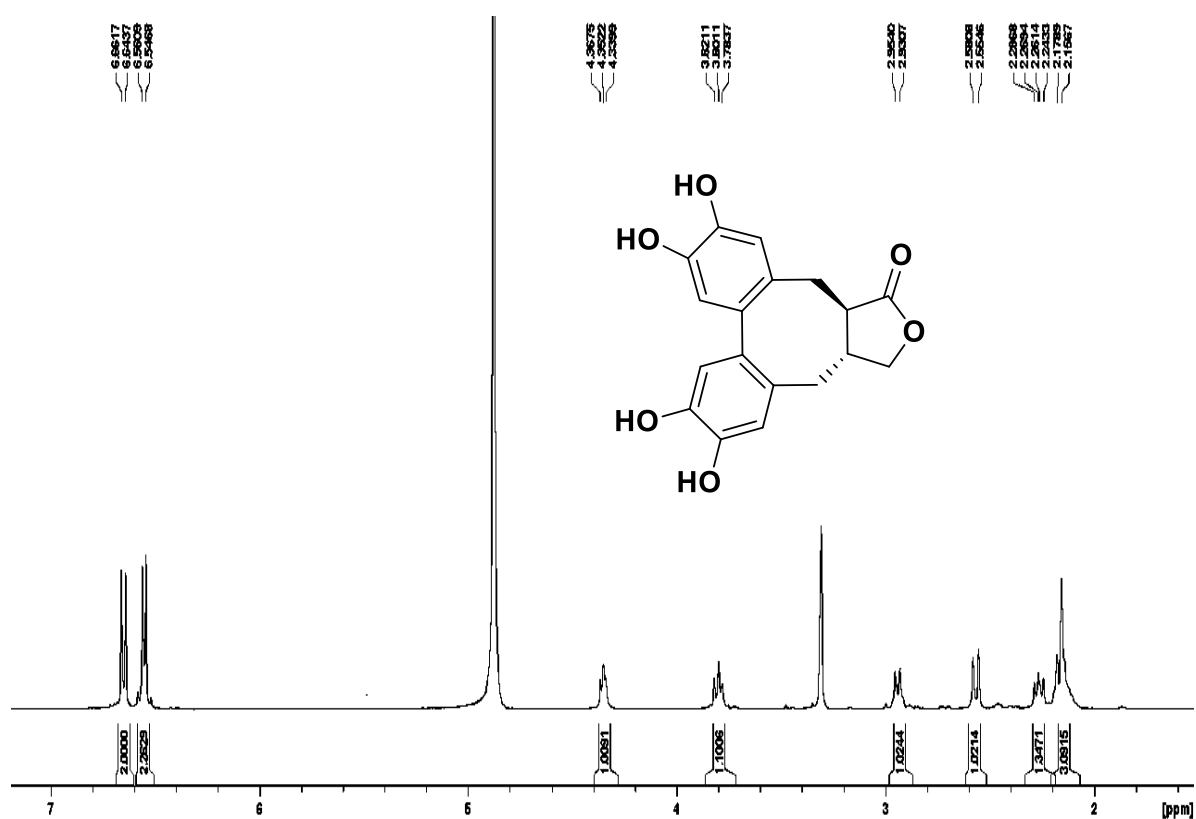
^1H -NMR (CDCl_3 , 500 MHz) of compound **15**.



^{13}C -NMR (CDCl_3 , 500 MHz) of compound **15**.



^1H -NMR (CDCl_3 , 500 MHz) of compound **16**.



^{13}C -NMR (CDCl_3 , 500 MHz) of compound **16**.

