

Chemistry & Biodiversity

Supporting Information

Neolignan Kadsurenin F Modulates Proteostatic Pathways and Possesses Potent Anti-Inflammatory Properties

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Supplementary Material

Table of contents

Figure S1. HPLC-MS spectrum of kadsurenin F

Figure S2. HPLC-online UV-spectrum of kadsurenin F

Figure S3. ¹H-NMR spectrum of kadsurenin F

Figure-S3-1. Magnification of the aromatic region of the ¹H-NMR-spectrum of kadsurenin F

Figure S4. ¹³C-NMR spectrum of kadsurenin F

Figure S5. ¹H,¹H-COSY-NMR spectrum of kadsurenin F

Figure S6. HSQC-NMR spectrum of kadsurenin F

Figure S7. HMBC-NMR spectrum of kadsurenin F

Figure S8. NOESY-NMR spectrum of kadsurenin F

Figure S9. ECD spectrum of kadsurenin F

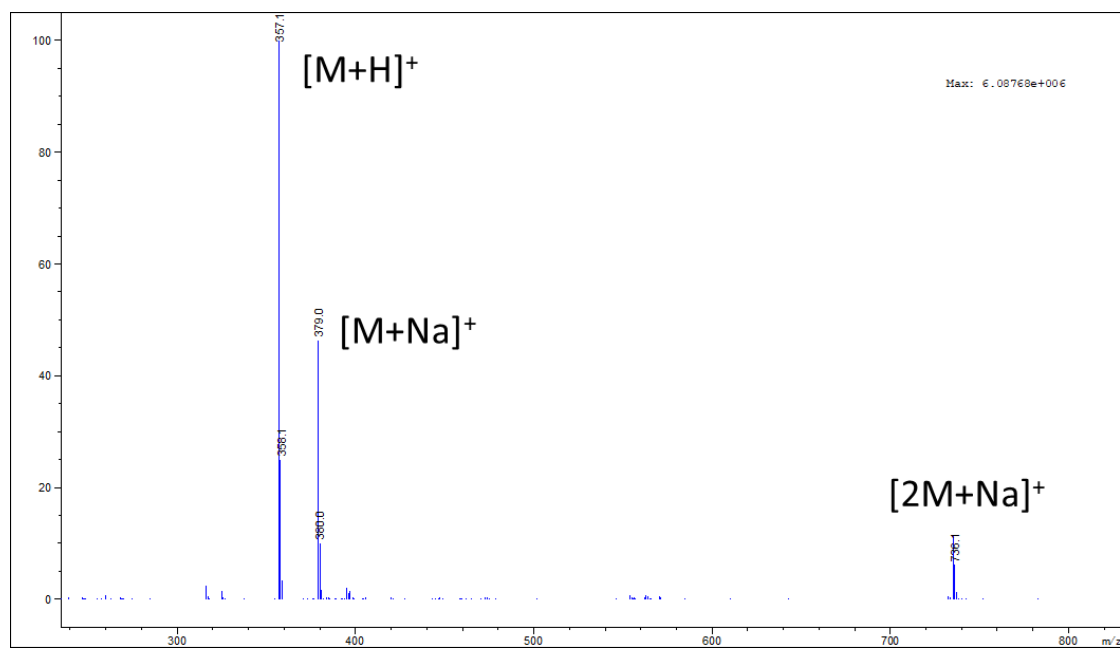


Figure S1. HPLC-MS spectrum of kadsurenin F; API-ESI, positive mode. For analytical conditions, see Experimental Section main article.

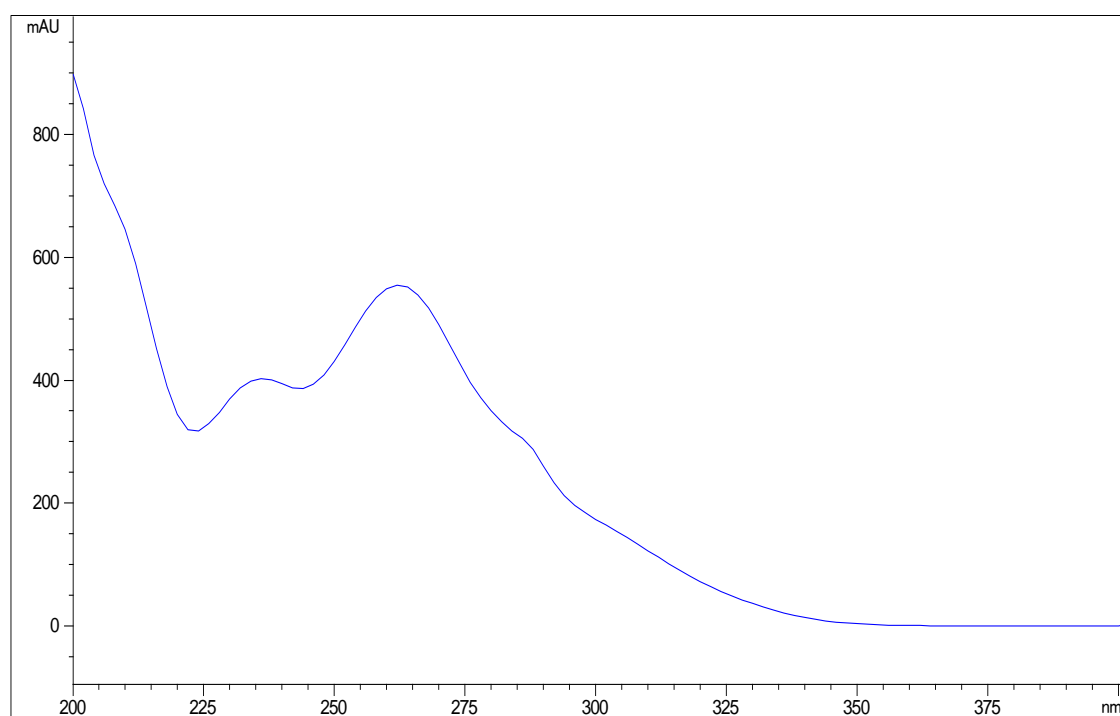


Figure S2. HPLC-online UV-spectrum of kadsurenin F. For analytical conditions, see Experimental Section main article.

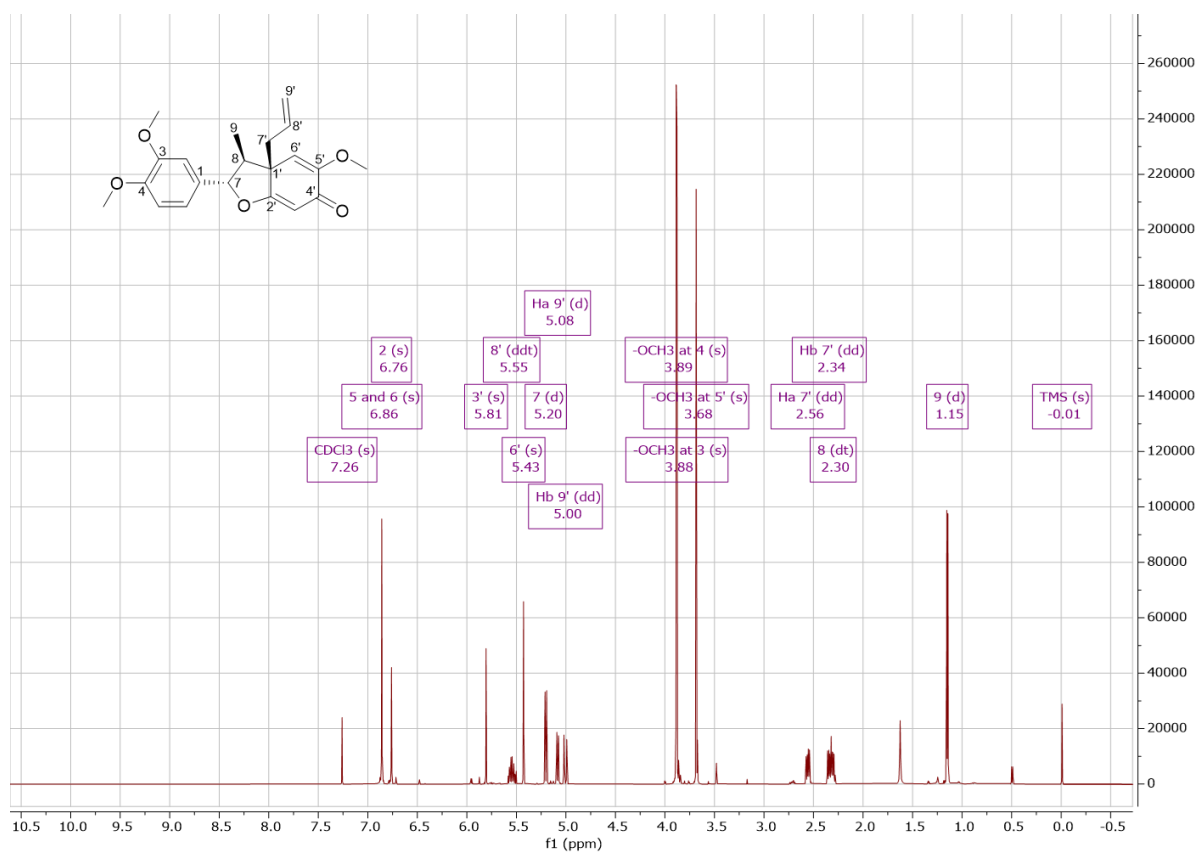


Figure S3. $^1\text{H-NMR}$ spectrum of kadsurenin F in CDCl_3 at 600.17 MHz.

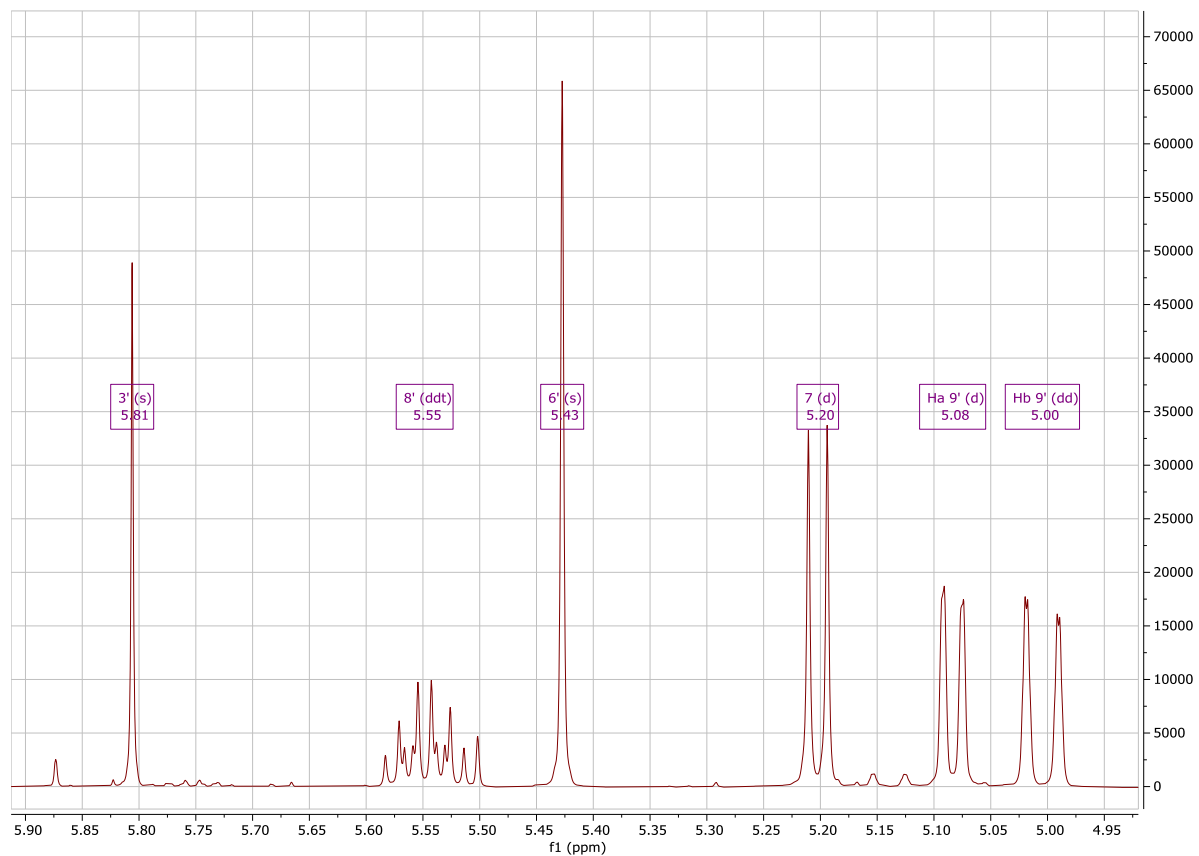


Figure-S3-1. Magnification of the aromatic region of the $^1\text{H-NMR}$ -spectrum of kadsurenin F in CDCl_3 at 600.17 MHz

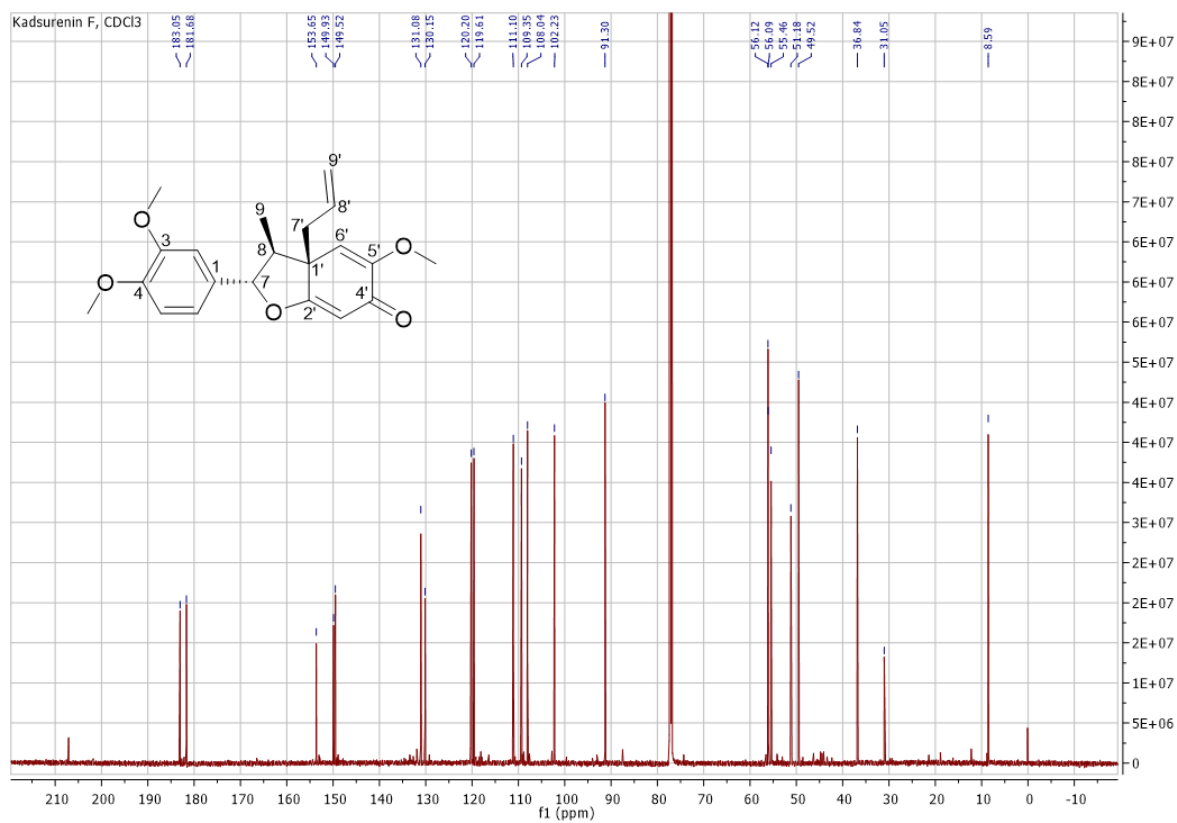


Figure S4. ¹³C-NMR spectrum of kadsurenin F in CDCl₃ at 150.91 MHz.

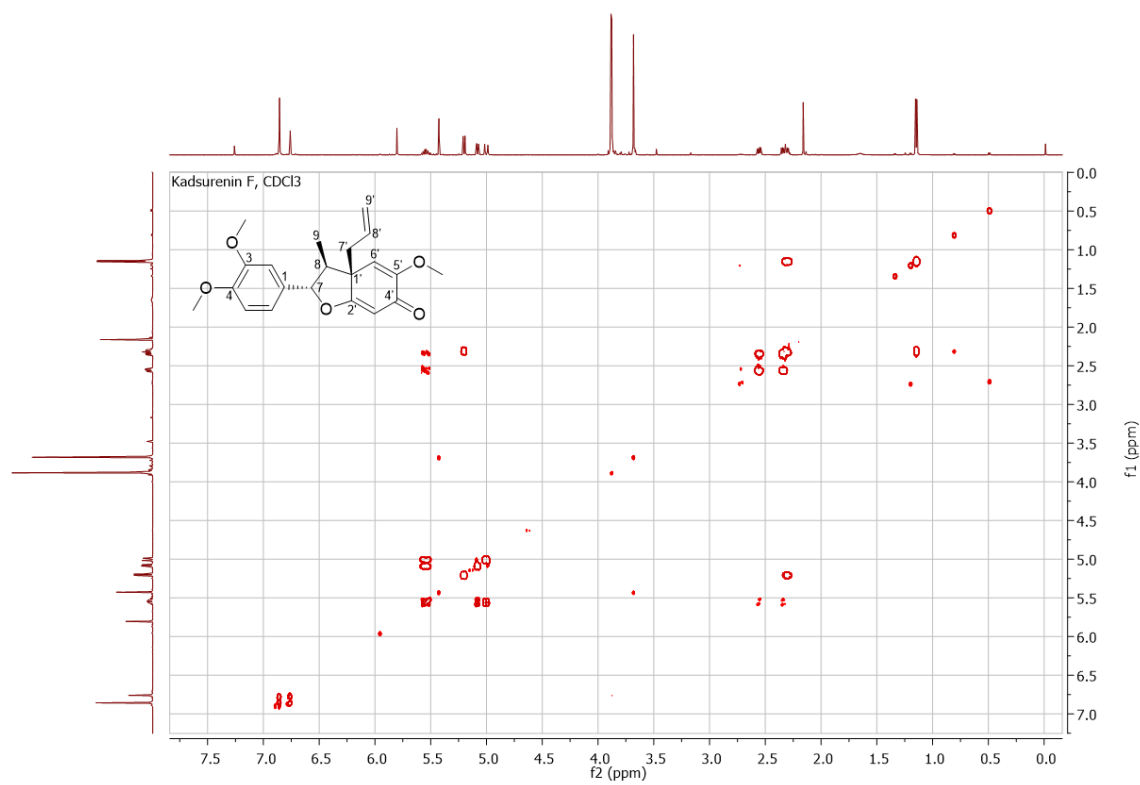


Figure S5. ¹H,¹H-COSY-NMR spectrum of kadsurenin F in CDCl₃ at 600.17 MHz.

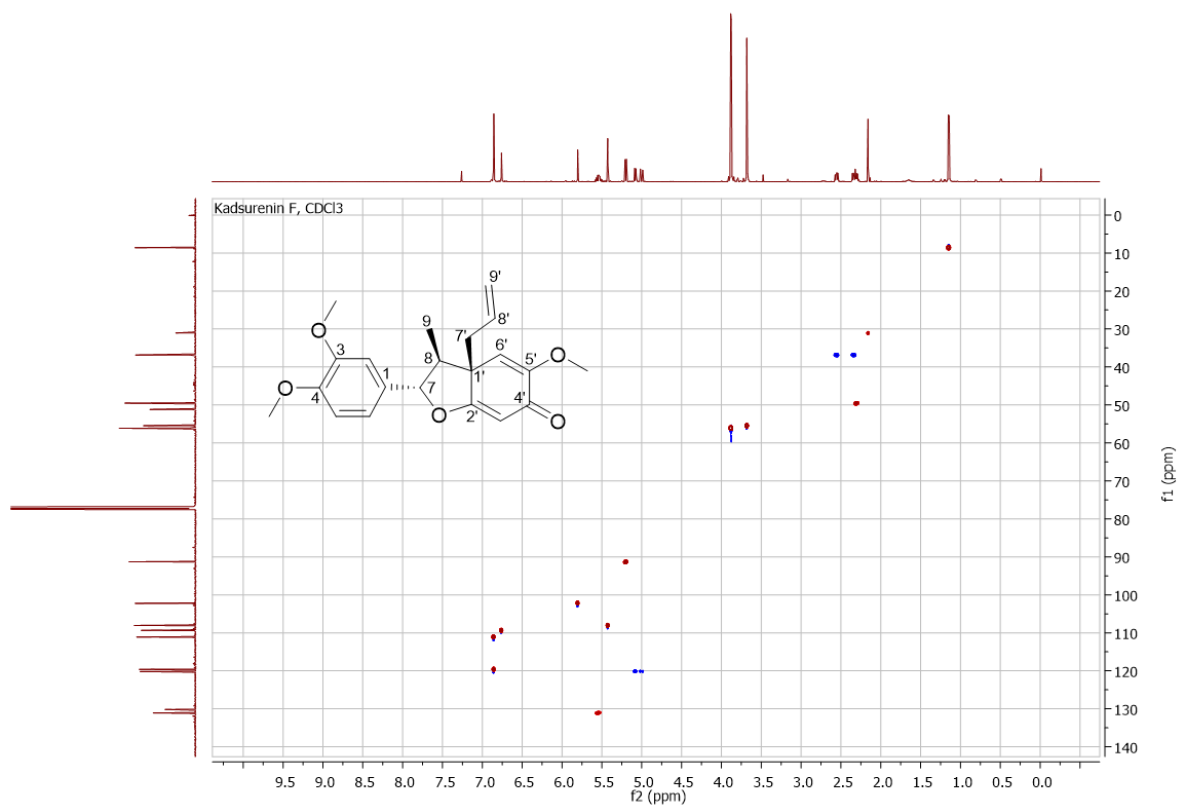


Figure S6. HSQC-NMR spectrum of kadsurenin F in CDCl₃ at 600.17/150.91 MHz.

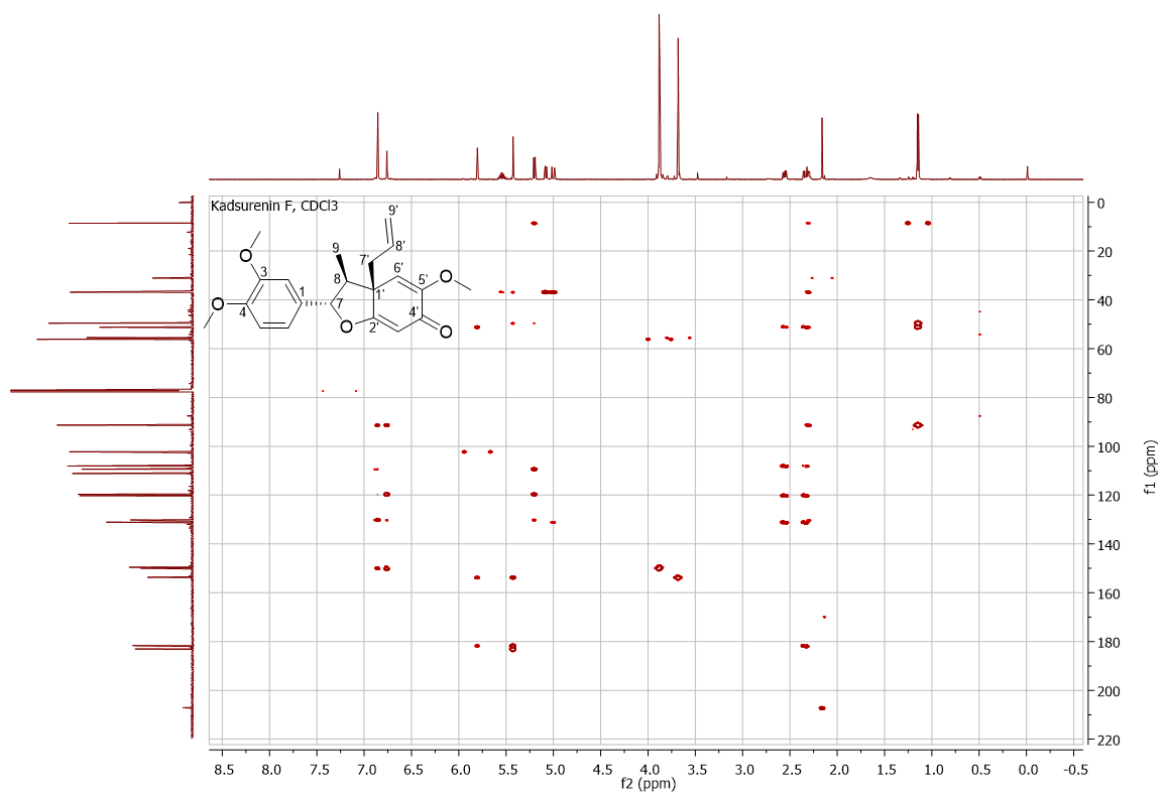


Figure S7. HMBC-NMR spectrum of kadsurenin F in CDCl₃ at 600.17/150.91 MHz.

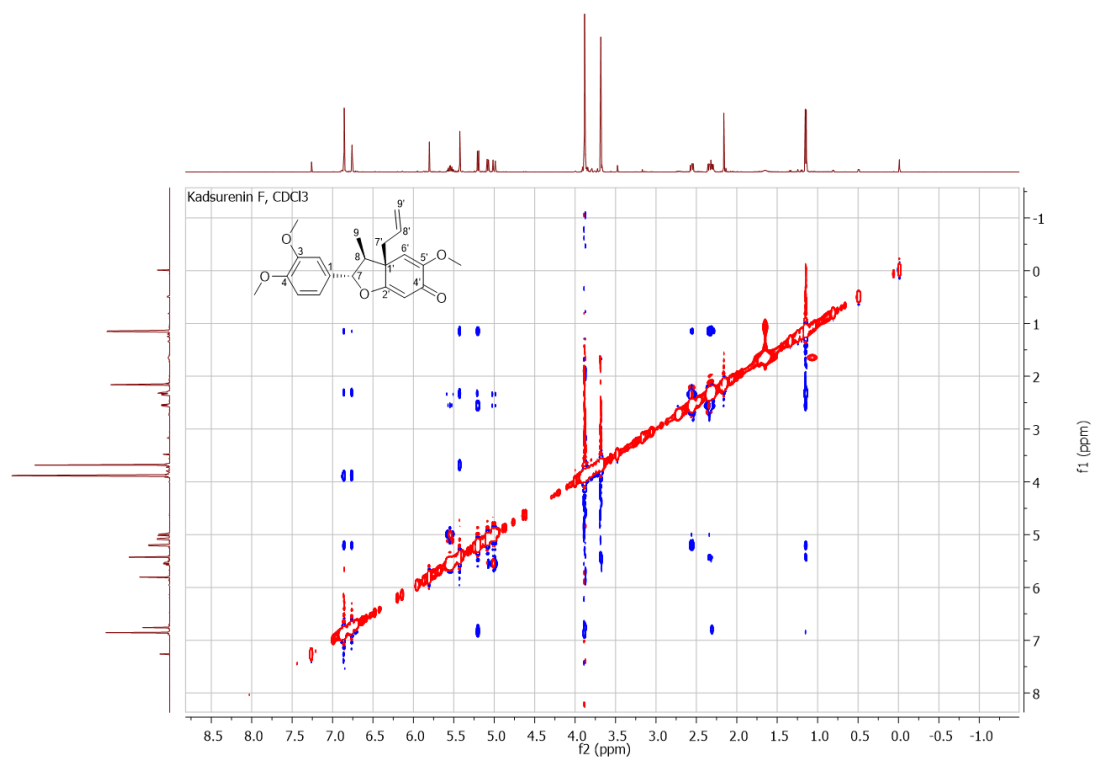


Figure S8. NOESY-NMR spectrum of kadsurenin F in CDCl_3 at 600.17 MHz.

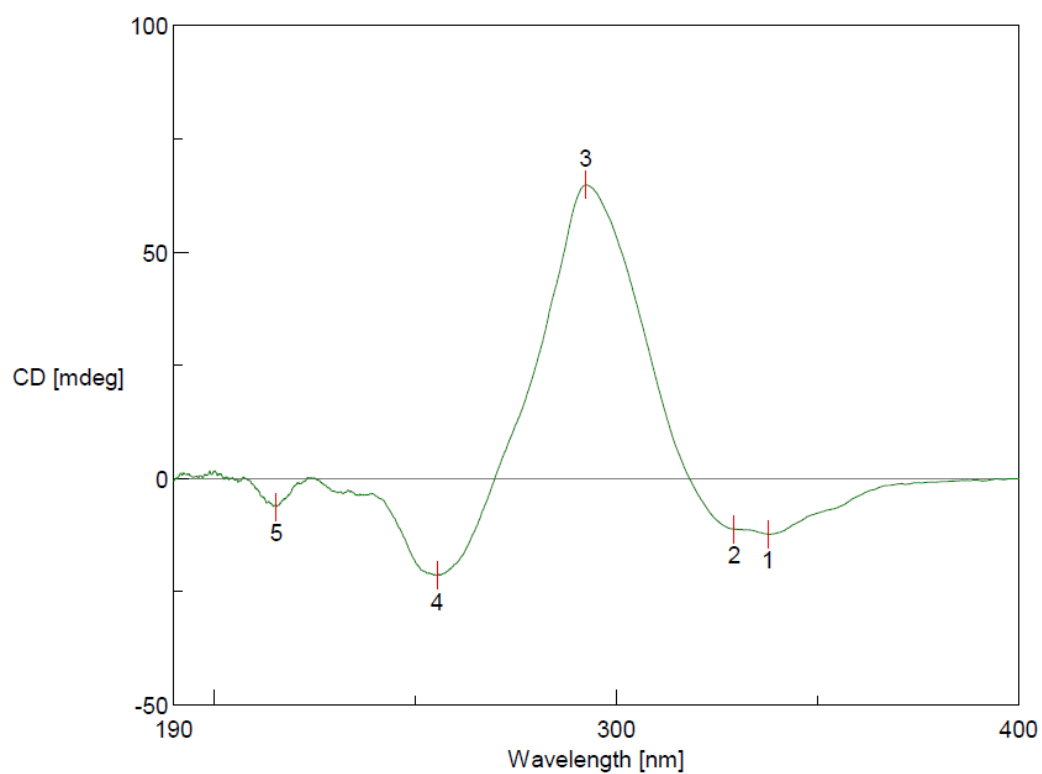


Figure S9. ECD spectrum of kadsurenin F in acetonitrile (71 $\mu\text{g/mL}$, corrected). Observed maxima, wavelength [nm]/CD [mdeg]: 337.7/-12.4329; 329.3/-11.3102; 292.4/64.8482; 255.5/-21.5166; 215.5/-6.33683.

Table 1. Experimental NMR data of kadsurenin F.

Position	¹ H-NMR data at 600.19 MHz in CDCl ₃ , J in Hz	¹³ C-NMR data at 150.91 MHz in CDCl ₃
1	---	130.15
2	6.76 s, 1H	109.35
3	---	149.52
4	---	149.93
5	6.86 br s, 1H	111.10
6	6.86 br s, 1H	119.61
7	5.20 d, J = 10.0 Hz, 1H	91.30
8	2.30 dt, J = 10.0, 6.7 Hz, 1H	49.52
9	1.15 d, J = 6.9 Hz, 3H	8.59
1'	---	51.18
2'	---	181.68
3'	5.81 s, 1H	102.23
4'	---	183.05
5'	---	153.65
6'	5.43 s, 1H	108.04
7'	H _a 2.56 dd, J = 13.4, 7.1 Hz H _b 2.34 dd, J = 13.2, 7.2 Hz	36.84
8'	5.55 ddt, J = 17.2, 10.2, 7.2 Hz, 1H	131.08
9'	H _a 5.08 br d, J = 10.1 Hz H _b 5.00 dd, J = 17.0, 1.6 Hz	120.20
-OCH ₃ at 3	3.879 s, 3H	56.08*
-OCH ₃ at 4	3.885 s, 3H	56.12*
-OCH ₃ at 5'	3.68 s, 3H	55.46
<i>*might be exchanged</i>		

